

# SOME THEORETICAL ASPECTS OF FIBRE SUSPENSION FLOWS

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by

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This thesis is dedicated to my mother and father.

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# Abstract

This thesis is concerned with properties of equations governing fibre suspensions. Of particular interest is the extent to which solutions, and their properties, depend on the type of closure used. For this purpose two closure rules are investigated: the linear and the quadratic closures. We show that the equations are consistent with the second law of thermodynamics, or dissipation inequality, when the quadratic closure is used. When the linear closure is used, a sufficient condition for consistency is that the particle number  $N_p$  satisfies  $N_p \leq 35/2$ . Likewise, flows are found to be monotonically stable for the quadratic closure, and for the linear closure with  $N_p \leq 35/2$ .

The second part of the thesis is concerned with one-dimensional problems, and their solution by finite element. The hyperbolic nature of the evolution equation for the orientation tensor necessitates a modification of the standard Galerkin-based approach. We investigate the conditions under which convergence is obtained, for unidirectional flows, with the use of the Streamline Upwind (SU) method, and the Streamline upwind Petrov/Galerkin (SUPG) method .

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# Chapter 1

## Introduction

The rheological behaviour of fibre suspensions, that is, suspensions of rigid particles in a fluid, is of great industrial interest. For example, in processes in which short-fibre composites are manufactured, the material to be processed generally takes the form of a fibre suspension; this is then moulded into the desired shape in highly automated processes such as injection or compression moulding, after which solidification yields the desired product.

The velocity fields in suspensions will generally depend on the orientation, distribution, and concentration of fibres, whose behaviour will also be affected by the fluid. The problem is thus highly coupled.

Theories regarding the mechanical properties of the composite exist. Once the fibre orientation state is known, one can use the existing theories to determine overall properties such as elastic modulus, thermal expansion, and strength when the matrix is solid; viscosity when the matrix is liquid; and thermal and electrical conductivity for both solid and liquid matrices [37].

There is a close and complex relationship between fibre orientation and flow characteristics, in suspensions. The fibres in a short-fibre composite are never aligned in the same direction, not even within a very small region. The issues of the distribution of fibres, their orientation, and how to model changes in orientation, are of central interest [17, 21, 37].

The use of orientation tensors as a means of characterising fibre orientation was suggested for the first time by Hand [21], and the idea has been subsequently investigated in some detail by Tucker and Advani [1, 2, 38]. This approach entails considering the fibres as a sample drawn from a finite population, and to characterising the orientation within that population by a probability density function. Another approach consists in computing a kind of average orientation by considering a small average volume within the composite [37]. The resulting mathematical model then incorporates both second- and fourth-order orientation tensors, which capture in a deterministic way information about fibre orientation. It is furthermore necessary to make an assumption, known as a closure approximation, about the dependence of the fourth-order tensor on that of second order, and a great many works have been devoted to the issue of how best to choose such closure approximations (see, for example, [2, 8, 22]).

Constitutive theories for fibre suspensions have received much attention. For suspensions in which the base fluid is Newtonian, for example, examples of key contributions are the works of Dinh and Armstrong [13], Leal and Hinch [26], and Tucker and Advani [37]. The constitutive equations generally take the form of a modification of the standard

Newtonian law, together with an evolution equation for the orientation tensor.

Given the complexity of the problem, it is natural that there have been investigations of numerical solutions to the equations for fibre suspension flows. Rosenberg et al [33] considered the numerical treatment of the processing of fibre suspensions, and presented results for the simulation of non-recirculating flows. Reddy and Mitchell [31] also presented details of a numerical investigation. Their work focussed on two features: first, the instabilities that can occur with the use of the linear closure approximation, and secondly, the behaviour of fibre suspension flows in domains which are characterised by abrupt changes in geometry. Because of the presence of the convective term in the evolution equation, they used an upwinding technique to construct finite element approximations.

There has been limited work on the qualitative properties of the equations governing fibre suspension flows. Galdi and Reddy [17] studied the issues of well-posedness of the problem of fibre suspension flows, and the existence and uniqueness of solutions to the equations governing of the fibre suspension flows. They found, in particular, that the rest state is unstable, in the sense of Liapounov, when the particle number exceeds  $35/2$ , in the case of the linear closure approximation.

This thesis is concerned with some theoretical aspects of the modelling of fibre suspension flows. The study uses the constitutive model based on orientation tensors, and its purpose is:

1. to investigate the circumstances under which the constitutive equations for fibre suspensions are consistent with the second law

of thermodynamics. The second law, in the form of a dissipation inequality, is thus regarded here as an inequality that must be satisfied by constitutive equations, for all admissible flows.

2. to study the energetic stability of fibre suspension flows.
3. to review finite element methods for problems in one space dimension that are of convective-diffusive type, and to apply the results of such approaches to a simple one-dimensional problem for fibre suspension flows.

We will focus on problems in which either the linear or quadratic closure approximations are used.

As many authors have shown, the finite element method applied to linear elliptic and parabolic problems leads to very satisfactory results, but this is not the case for hyperbolic problems such as convection-diffusion problems with small or vanishing diffusion. While standard finite element methods do converge, the results are not satisfactory for situations in which the exact solution is not smooth. To avoid such problems, it is necessary to modify the standard method, and various such modifications have been proposed: these include the discontinuous Galerkin, streamline upwind Petrov-Galerkin, and the streamline upwind methods [24].

It will be seen that the evolution equation for the orientation tensor contains the convective term  $(\mathbf{v} \cdot \nabla) \mathbf{A}$ . Under this circumstance, it is inadvisable to use the standard finite element method, to solve the fibre suspension problem. It will be seen, in particular, that the order of the estimated error between the exact and the approximate solutions

found using the standard Galerkin is sub-optimal, while the use of one of the non-standard finite element methods leads to convergence at the optimal rate. The outline of the thesis is as follows.

Chapter 2 begins with a review of those aspects of fluid mechanics that are useful in the present work. The chapter contains details of the equations for balance of mass, of linear momentum, and of angular momentum. The Navier- Stokes equations are also reviewed.

Details of the continuum theory of fibre suspensions are presented. Included is a discussion of the orientation tensors, and various closure approximations. The evolution equation for orientation and the constitutive equation for the stress are discussed.

Chapter 3 is devoted to thermodynamic aspects of fibre suspension flows. The second law, in the form of the Clausius-Duhem inequality is reviewed, and the consistency of the constitutive equations with the second law are investigated, for the linear and quadratic closures. Also discussed in this chapter is the issue of energetic stability.

Chapter 4 deals with unidirectional flow. We study the exact solution of the unidirectional flow problem for fibre suspensions.

In chapter 5, we review the main aspects of the finite element method in one space dimension, in the context of a model convection-diffusion problem. We investigate the issue of convergence for the Galerkin method, the streamline upwind/ Petrov-Galerkin formulation [6, 24] and the streamline upwind method [12, 29]; these results are applied to the evolution equation for fibre suspension flows in one space dimension.

This thesis ends with concluding remarks in Chapter 6, while some basic mathematical results are collected in the Appendix.

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## Chapter 2

# Governing Equations

In this chapter we present the equations that govern the behaviour of fibre suspensions. We begin in Section 2.1 with the equations for conservation of mass and linear momentum; these lead to the continuity equation and Cauchy's equation of motion, respectively, which both apply to all continuous media. We also give the equation of balance of angular momentum, which leads to the symmetry of the stress tensor  $\mathbf{T}$ . Then in Section 2.2 we discuss fibre suspensions, and in particular review the constitutive theory for such fluids that is based on the notion of orientation tensors.

**Notation.** In this and later chapters we denote vectors and tensors by bold-face letters. The components  $v_i$  of a vector  $\mathbf{v}$  and  $T_{ij}$  of a second-order tensor  $\mathbf{T}$  are always referred to a fixed cartesian basis, unless otherwise stated. The same applies to the components  $\mathcal{A}_{ij}$  of a fourth-order tensor  $\mathcal{A}$ . The summation convention of Einstein for repeated indices is always applied.



The inner product of two vectors  $\mathbf{v}$  and  $\mathbf{w}$  is defined by

$$\mathbf{v} \cdot \mathbf{w} = v_i w_i,$$

and the inner product of two second-order tensors  $\mathbf{S}$  and  $\mathbf{T}$  by

$$\mathbf{S} : \mathbf{T} = S_{ij} T_{ij}.$$

The magnitude of a tensor  $\mathbf{T}$  is defined by

$$|\mathbf{T}| = (\mathbf{T} : \mathbf{T})^{1/2}.$$

The gradient  $\nabla \mathbf{v}$  of a vector field  $\mathbf{v}$  is a second-order tensor with components

$$(\nabla \mathbf{v})_{ij} = \frac{\partial v_i}{\partial x_j}.$$

The divergence of a vector field  $\mathbf{v}$  is the scalar field defined by

$$\operatorname{div} \mathbf{v} = \operatorname{tr} \nabla \mathbf{v} = \frac{\partial v_i}{\partial x_i}.$$

The divergence of a second-order tensor field  $\mathbf{T}$  is a vector field defined by

$$\operatorname{div} \mathbf{T} = \frac{\partial T_{ij}}{\partial x_j} \mathbf{e}_i,$$

where  $\mathbf{e}_j$  are the unit basis vectors corresponding to the cartesian coordinate system.

The Laplacian of a vector field is the vector field defined by

$$\Delta \mathbf{v} = \frac{\partial^2 v_i}{\partial x_j \partial x_j} \mathbf{e}_i.$$

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The divergence theorem of Gauss states that, if  $\Omega$  is a closed domain with smooth boundary  $\Gamma$ , then

$$\int_{\Omega} \operatorname{div} \mathbf{v} \, dV = \int_{\Gamma} \mathbf{v} \cdot \mathbf{n} \, dS \quad (2.1)$$

for any smooth vector field  $\mathbf{v}$  and

$$\int_{\Omega} \operatorname{div} \mathbf{T} \, dV = \int_{\Gamma} \mathbf{T} \mathbf{n} \, dS \quad (2.2)$$

for any smooth tensor field  $\mathbf{T}$ .

### 2.1 Balance of mass, of linear momentum, and of angular momentum

#### 2.1.1 Conservation of mass: the continuity equation

Let  $\Omega$  be a bounded domain in  $\mathbb{R}^n$  ( $n = 1, 2, 3$ ) occupied by a fluid with boundary  $\Gamma$ . Points in  $\Omega$  are denoted by the vector  $\mathbf{x}$ , with components  $x_i$ . The fluid has density  $\rho(\mathbf{x}, t)$  and velocity  $\mathbf{v}(\mathbf{x}, t)$ , where  $t$  denotes time. Then the law of balance of mass states that the rate of change of mass of the fluid is zero. That is,

$$\frac{d}{dt} \int_{\Omega} \rho \, dV = 0. \quad (2.3)$$

Now  $\Omega$  is a material region, and is therefore time-dependent, so that the time derivative cannot be taken inside the integral. We can, however, transform to a fixed reference domain  $\Omega_0$ , and then commute the derivative with the integral over  $\Omega_0$ .

Let  $J$  denote the Jacobian of the transformation from  $\Omega$  to  $\Omega_0$ ; then the material rate of change of  $J$  is given by

$$\frac{DJ}{Dt} = J \operatorname{div} \mathbf{v} \quad (2.4)$$

(see, for example, [3]). Here  $D/Dt$  denotes the material derivative, defined for a scalar field  $\rho$  by

$$\frac{D\rho}{Dt} = \frac{\partial \rho}{\partial t} + \mathbf{v} \cdot \nabla \rho.$$

The material derivative is the rate of change of a quantity following the fluid, whereas the partial derivative  $\partial \rho / \partial t$  measures the rate of change at a spatial point.

Denoting the volume element in  $\Omega_0$  by  $dV_0$ , we have

$$\begin{aligned} 0 &= \frac{d}{dt} \int_{\Omega} \rho \, dV \\ &= \frac{d}{dt} \int_{\Omega_0} \rho \, J dV_0 \\ &= \int_{\Omega_0} \frac{D}{Dt} [\rho J] \, dV_0 \\ &= \int_{\Omega_0} [\dot{\rho} J + \rho J \operatorname{div} \mathbf{v}] \, dV_0 \\ &= \int_{\Omega_0} [\dot{\rho} + \rho \operatorname{div} \mathbf{v}] \, J dV_0 \\ &= \int_{\Omega} [\dot{\rho} + \rho \operatorname{div} \mathbf{v}] \, dV, \end{aligned}$$

where  $\dot{\rho}$  denotes the material derivative of  $\rho$ .

Since  $\Omega$  is an arbitrary region, this implies that

$$\frac{D\rho}{Dt} + \rho \operatorname{div} \mathbf{v} = 0. \quad (2.5)$$

Equation (2.5) is known as the *continuity equation*.

We shall be dealing only with *incompressible* fluids, for which the volume of any arbitrary subregion of the fluid never changes. Under these conditions the material derivative of the density vanishes, and the continuity equation becomes the incompressibility condition

$$\operatorname{div} \mathbf{v} = 0. \quad (2.6)$$

### 2.1.2 Balance of linear momentum

The law of balance of linear momentum states that the rate of change of linear momentum of the fluid occupying the region  $\Omega$  equals the total force applied to that fluid. The fluid is subjected to two types of forces: (a) a body force  $\mathbf{b}$  per unit mass, which acts on the volume of the fluid, and (b) a surface traction  $\mathbf{t}$  per unit area, which acts on the bounding surface. Then, mathematically, balance of linear momentum states that

$$\frac{d}{dt} \int_{\Omega} \rho \mathbf{v} \, dV = \int_{\Omega} \rho \mathbf{b} \, dV + \int_{\Gamma} \mathbf{t} \, dS. \quad (2.7)$$

Once again using (2.4), the left hand side of (2.7) can be simplified according to

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} \rho \mathbf{v} \, dV &= \int_{\Omega_0} \frac{D}{Dt} [\rho \mathbf{v} J] \, dV_0 \\ &= \int_{\Omega_0} [\dot{\mathbf{v}} \rho J + \rho \dot{\mathbf{v}} J + \rho \mathbf{v} \dot{J}] \, dV_0 \\ &= \int_{\Omega_0} [(\dot{\rho} + \rho \operatorname{div} \mathbf{v}) \mathbf{v} + \rho \dot{\mathbf{v}}] \, dV \\ &= \int_{\Omega_0} \rho \dot{\mathbf{v}} \, dV, \end{aligned} \quad (2.8)$$

because  $\dot{\rho} + \rho \operatorname{div} \mathbf{v} = 0$  by the continuity equation.

Next we have to simplify the righthand side of (2.7). For this we will need Cauchy's theorem, according to which a second-order tensor, called the stress tensor  $\mathbf{T}$ , exists, with the property that the surface traction  $\mathbf{t}$  on a surface with unit normal  $\mathbf{n}$  is given by

$$\mathbf{t} = \mathbf{T}\mathbf{n}.$$

The second term of the right hand of (2.7) is therefore, using also (2.2),

$$\begin{aligned} \int_{\Gamma} \mathbf{t} \, dS &= \int_{\Gamma} \mathbf{T}\mathbf{n} \, dS \\ &= \int_{\Omega} \operatorname{div} \mathbf{T} \, dV. \end{aligned}$$

Equation (2.7) now becomes

$$\int_{\Omega} \left( \rho \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} - \operatorname{div} \mathbf{T} - \rho \mathbf{b} \right) dV = 0. \quad (2.9)$$

Since the region  $\Omega$  is arbitrary, we obtain Cauchy's equation of motion

$$\rho \frac{D \mathbf{v}}{Dt} - \operatorname{div} \mathbf{T} = \rho \mathbf{b}. \quad (2.10)$$

A relevant example of a fluid is that of an incompressible Newtonian fluid, for which the stress is given by

$$\mathbf{T} = -p\mathbf{I} + 2\mu\mathbf{D}, \quad (2.11)$$

where  $p$  is a hydrostatic pressure,  $\mu$  is the dynamic viscosity, and  $\mathbf{D}$  is the deformation rate tensor, defined by

$$\mathbf{D} = \frac{1}{2} (\nabla \mathbf{v} + (\nabla \mathbf{v})^T), \quad (2.12)$$

and  $\mathbf{A}^T$  indicates the transpose of a tensor  $\mathbf{A}$ . Substitution of (2.11) in (2.10) and recollection of the incompressibility condition (2.6) leads to the *Navier-Stokes equations*

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} - \nu \Delta \mathbf{v} + \frac{1}{\rho} \nabla p = \mathbf{b}, \quad (2.13)$$

$$\operatorname{div} \mathbf{v} = 0. \quad (2.14)$$

in which  $\nu = \mu/\rho$  is the kinematic viscosity.

### 2.1.3 Balance of angular momentum

The law of balance of angular momentum states that the rate of change of angular momentum of the fluid occupying the region  $\Omega$  equals the total moment. As above, we suppose that the fluid is subjected to two types of forces: (a) a body force  $\mathbf{b}$  per unit mass, which acts on the volume of the fluid, and (b) a surface traction  $\mathbf{t}$  per unit area, which acts on the bounding surface. Then, mathematically, balance of angular momentum states that

$$\frac{d}{dt} \int_{\Omega} \mathbf{x} \times \rho \mathbf{v} dV = \int_{\Omega} \mathbf{x} \times \rho \mathbf{b} dV + \int_{\Gamma} \mathbf{x} \times \mathbf{t} dA. \quad (2.15)$$

We now show that the law of balance of angular momentum implies the symmetry of the stress tensor  $\mathbf{T}$ .

$$\begin{aligned} \text{The LHS of (2.15)} &= \int_{\Omega_0} \frac{D}{Dt} (\rho \mathbf{x} \times \mathbf{v} \cdot \mathbf{J}) dV_0 \\ &= \int_{\Omega_0} [\dot{\rho} \mathbf{x} \times \mathbf{v} \cdot \mathbf{J} + \rho \dot{\mathbf{x}} \times \mathbf{v} \cdot \mathbf{J} + \rho \mathbf{x} \times \dot{\mathbf{v}} \cdot \mathbf{J}] dV_0 \\ &\quad + \int_{\Omega_0} [\rho \mathbf{x} \times \mathbf{v} \cdot \dot{\mathbf{J}}] dV_0 \end{aligned}$$

$$\begin{aligned}
&= \int_{\Omega_0} [\dot{\rho} \mathbf{x} \times \mathbf{v} \cdot \mathbf{J} + \rho \mathbf{v} \times \mathbf{v} J + \rho \mathbf{x} \times \mathbf{a} J] dV_0 \\
&\quad + \int_{\Omega_0} [\rho \mathbf{x} \times J \operatorname{div} \mathbf{v}] dV_0. \tag{2.16}
\end{aligned}$$

The first and the fourth terms on the RHS of (2.16) give

$$J(\mathbf{x} \times \mathbf{v})(\dot{\rho} + \rho \operatorname{div} \mathbf{v}) = 0, \tag{2.17}$$

from the continuity equation.

The second term on the RHS of (2.16) is zero, because  $\mathbf{v} \times \mathbf{v} = \mathbf{0}$ . So, the LHS of (2.15) is

$$\int_{\Omega} \rho \mathbf{x} \times \mathbf{a} J dV. \tag{2.18}$$

The second term of the RHS of (2.15) is

$$\begin{aligned}
\int_{\Gamma} \varepsilon_{ijk} x_i t_j \mathbf{e}_k dA &= \int_{\Gamma} \varepsilon_{ijk} x_i T_{j\ell} n_{\ell} \mathbf{e}_k dA \\
&= \int_V \frac{\partial}{\partial x_{\ell}} [\varepsilon_{ijk} x_i T_{j\ell}] \mathbf{e}_k dV \\
&= \int_V \varepsilon_{ijk} [x_{i,\ell} T_{j\ell} + x_i T_{j\ell,\ell}] \mathbf{e}_k dV \\
&= \int_V \varepsilon_{ijk} [T_{ji} + x_i T_{j,\ell\ell}] \mathbf{e}_k dV \\
&= \int_V (\varepsilon_{ijk} T_{ji} \mathbf{e}_k + \mathbf{x} \times \operatorname{div} \mathbf{T}) dV.
\end{aligned}$$

We now collect all the terms, so that (2.15) can be written as

$$\int_{\Omega} [(\rho \mathbf{x} \times \mathbf{a} - \mathbf{x} \times \operatorname{div} \mathbf{T} - \mathbf{x} \times \rho \mathbf{b}) - \varepsilon_{ijk} T_{ji} \mathbf{e}_k] dV = 0,$$

or

$$\int_{\Omega} \varepsilon_{ijk} T_{ji} \mathbf{e}_k dV = 0, \tag{2.19}$$

since the term between brackets in (2.19) is just

$$\mathbf{x} \times (\rho \mathbf{a} - \operatorname{div} \mathbf{T} - \rho \mathbf{b}) = \mathbf{0} ,$$

by using the law of balance of linear momentum. Equation (2.19) implies that

$$\varepsilon_{ijk} T_{ji} = 0 , \quad (2.20)$$

since  $\Omega$  is an arbitrary region. From this equation it is easy to deduce that

$$T_{ij} = T_{ji} ,$$

that is, the stress tensor  $\mathbf{T}$  is symmetric.

## 2.2 Fibre suspensions

Consider a Newtonian fluid in which fibres are distributed throughout the volume of the fluid. Such a fluid is known as a fibre suspension. Each fibre is assumed to be axisymmetric-either cylindrical or ellipsoidal. The orientation of a fibre is described by the unit vector  $\mathbf{p}$ , as shown in Figure 2.1.

A fibre suspension can be characterised by the fibre volume fraction  $c$ , that is, the ratio of the volume of fibres to the total volume, and the fibre aspect ratio  $r = \frac{\ell}{d}$ , in which  $\ell$  and  $d$  are respectively the fibre length and diameter (see Figure 2.1).

A suspension is said to be

$$\left. \begin{array}{l} \text{dilute} \\ \text{semi-dilute} \\ \text{concentrated} \end{array} \right\} \quad \text{if} \quad \left\{ \begin{array}{l} cr^2 < 1 \\ 1 < cr^2 < r \\ 1 < cr \end{array} \right. \quad (2.21)$$



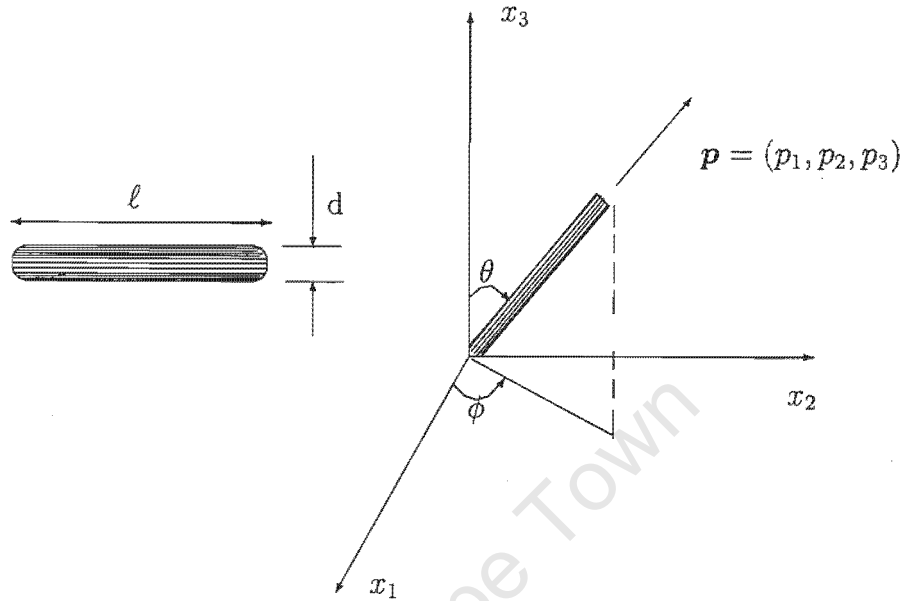


Figure 2.1: single fibre orientation

We will consider dilute and semi-dilute suspensions, for which fibres have a low probability of making contact, though the fibres and the fluid motion are coupled.

Fibres are never generally aligned in the same direction, not even within a very small region, and it is difficult to predict how the orientation of fibres will depend on the velocity field of the fluid. It is also unrealistic to try to describe the orientation of each fibre, and under this circumstance, a feasible approach is to describe fibre orientation in a probabilistic manner.

Consider (see, for example, [1, 2, 37, 38]), a representative volume of the fibre suspension. We characterize the fibre orientation in this

volume by a probability density function  $\psi(\theta, \phi)$  or  $\psi(\mathbf{p})$ ; the probability of any given fibre lying in the range between  $\theta_1$  and  $\theta_1 + d\theta$ , and between  $\phi_1$  and  $\phi_1 + d\phi$ , is given by

$$P(\theta_1 \leq \theta \leq \theta_1 + d\theta, \phi_1 \leq \phi \leq \phi_1 + d\phi) = \psi(\theta_1, \phi_1) \sin \theta_1 d\theta d\phi. \quad (2.22)$$

A constitutive theory based on the concept of orientation tensors will be used. Fundamental to the definition of these tensors is the averaging operator  $\langle \cdot \rangle$ , defined by

$$\langle f \rangle = \int_{S^1} f(\mathbf{p}) \psi(\mathbf{p}) d\mathbf{p} \equiv \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} f(\theta, \phi) \psi(\theta, \phi) \sin \theta d\theta d\phi$$

where  $(\theta, \phi)$  are spherical coordinates. It follows from the definition that

$$\int \psi(\mathbf{p}) d\mathbf{p} = 1. \quad (2.23)$$

**Definition 2.1** (a) The orientation tensor  $\mathbf{A}$  of first order is defined by

$$\mathbf{A} = \langle \mathbf{p} \rangle, \quad (2.24)$$

(b) The orientation tensor  $\mathbf{A}^m$  of order  $m$  is defined by

$$\mathbf{A}^m = \langle \mathbf{p} \otimes \mathbf{p} \otimes \dots \rangle, \quad (2.25)$$

the product being taken over  $m$  vectors  $\mathbf{p}$ . In component form,

$$A_{ijk\dots}^m = \langle p_i p_j p_k p_l \dots \rangle.$$

The choice of direction of  $\mathbf{p}$  is arbitrary, since the orientation of a fibre does not change if one substitutes

$$\mathbf{p} \text{ for } -\mathbf{p} \quad (2.26)$$

or

$$\theta \text{ by } \pi - \theta \text{ and } \phi \text{ by } \phi + \pi \quad (2.27)$$

**Theorem 2.1** *All orientation tensors of odd order are zero.*

**Proof.** Consider for convenience the case of the orientation tensor of order three. We have

$$\begin{aligned} -A_{ijk}^m &= -\langle p_i p_j p_k \rangle \\ &= \langle -p_i (-p_j) (-p_k) \rangle \\ &= \langle p_i p_j p_k \rangle, \text{ using (2.26)} \\ &= A_{ijk}^m \end{aligned}$$

since the integration of  $\mathbf{p}$  over the unit sphere is sign-invariant. In the same way we can show that  $A_{ijk}^m = 0$  for  $m$  odd.

Thus it is only the even-order orientation tensors that are relevant, as we said earlier. We will be concerned in particular with the second- and fourth-order tensors, which will be denoted henceforth by  $\mathbf{A}$  and  $\mathcal{A}$ , respectively. That is,

$$\begin{aligned} A_{ij} &= \langle p_i p_j \rangle, \\ \mathcal{A}_{ijkl} &= \langle p_i p_j p_k p_l \rangle. \end{aligned} \quad (2.28)$$

Some properties of these tensors are summarised in the following theorem.

**Theorem 2.2** (a) *The tensor  $\mathbf{A}$  has the following two properties:*

$$A_{ji} = A_{ij} \text{ (symmetry), } A_{ii} = 1. \quad (2.29)$$

(b) *The tensor  $\mathcal{A}$  satisfies the following properties:*

$$\mathcal{A}_{ijkl} = \mathcal{A}_{jikl} = \mathcal{A}_{kijl} = \mathcal{A}_{likj} = \mathcal{A}_{klij}, \text{ etc. ,} \quad (2.30)$$

$$\mathcal{A}_{ijkk} = A_{ij}. \quad (2.31)$$

**Proof.** (a) We have

$$\begin{aligned} A_{ij} &= \langle p_i p_j \rangle \\ &= \int p_i p_j \psi(\mathbf{p}) d\mathbf{p} \\ &= \int p_j p_i \psi(\mathbf{p}) d\mathbf{p} \\ &= \langle p_j p_i \rangle \\ &= A_{ji}. \end{aligned}$$

Secondly,

$$\begin{aligned} A_{ii} &= \langle p_i p_i \rangle \\ &= \int p_i p_i \psi(\mathbf{p}) d\mathbf{p} \\ &= \int \psi(\mathbf{p}) d\mathbf{p} \\ &= 1, \text{ using (2.23).} \end{aligned}$$

(b) We have

$$\begin{aligned} \mathcal{A}_{ijkl} &= \langle p_i p_j p_k p_l \rangle \\ &= \int p_i p_j p_k p_l \psi(\mathbf{p}) d\mathbf{p} \\ &= \int p_j p_i p_k p_l \psi(\mathbf{p}) d\mathbf{p} \\ &= \mathcal{A}_{jikl}. \end{aligned}$$

The other symmetries are established in the same way.

Finally,

$$\begin{aligned}\mathcal{A}_{ijkk} &= \int p_i p_j p_k p_k \psi(\mathbf{p}) d\mathbf{p} \\ &= \int p_i p_j \psi(\mathbf{p}) d\mathbf{p} \\ &= A_{ij}.\end{aligned}$$

### 2.2.1 Evolution equation for orientation tensors

The basis for deriving the evolution equation for orientation tensors is the work of Jeffery [23], who studied the behaviour of a single rigid ellipsoid in an infinite body of Newtonian fluid. The motion of a single fibre is given by the equation [1, 2]

$$\dot{\mathbf{p}} = \mathbf{W}\mathbf{p} + \lambda \left[ \mathbf{D}\mathbf{p} - (\mathbf{p} \cdot \mathbf{D}\mathbf{p})\mathbf{p} \right] - D_r \frac{1}{\psi} \frac{\partial \psi}{\partial \mathbf{p}}. \quad (2.32)$$

Here  $\mathbf{W}$  is the spin tensor, a skew-symmetric tensor defined by

$$\mathbf{W} = \frac{1}{2}(\nabla \mathbf{v} - \nabla \mathbf{v}^T), \quad (2.33)$$

$\mathbf{D}$  is the deformation rate tensor, which has been defined earlier,  $D_r$  is the rotary diffusivity, and  $\lambda$  is a material constant that depends on the fibre aspect ratio  $r$ :

$$\lambda = \frac{r^2 - 1}{r^2 + 1}. \quad (2.34)$$

For spherical particles  $\lambda = 0$  and  $\lambda \rightarrow 1$  in the case of a slender body.

The constant  $D_r$  depends on the size of the particles and the viscosity

and temperature of the suspending fluid. In the case of  $D_r$  equal to zero, (2.32) is Jeffery's equation for the motion of rigid ellipsoidal particle in a Newtonian fluid [1, 37]. Several workers have chosen Jeffery's equation for the case of dilute suspensions, for which  $D_r$  is very small. Folgar and Tucker [15, 37] have proposed a model in which the diffusivity is approximated in terms of the flow by

$$D_r = 2\sqrt{2}C_I|\mathbf{D}|,$$

where  $|\mathbf{D}|$  is, as usual, the magnitude of the deformation rate tensor and  $C_I$  is an empirical material constant called the *interaction coefficient*.

Since the fibres change orientation in time, so does  $\psi$  too change in time, and the probability density must satisfy the continuity condition [1]

$$\frac{D\psi}{Dt} = -\frac{\partial}{\partial \mathbf{p}}(\psi \dot{\mathbf{p}}). \quad (2.35)$$

By using the equations (2.32), (2.35), and (2.28) we obtain the evolution equation for the orientation tensor  $\mathbf{A}$  in the form

$$\frac{D\mathbf{A}}{Dt} + \mathbf{A}\mathbf{W} - \mathbf{W}\mathbf{A} - \lambda(\mathbf{D}\mathbf{A} + \mathbf{A}\mathbf{D} - 2\mathbf{A}\mathbf{D}) - D_r(\mathbf{I} - n\mathbf{A}) = \mathbf{0}, \quad (2.36)$$

for a problem posed in  $\mathbb{R}^n$ .

### 2.2.2 Closure approximations

The evolution equation for  $\mathbf{A}$  contains the tensor  $\mathcal{A}$ , and it can be shown (Tucker and Advani [2]) that the evolution equation for an orientation tensor  $\mathbf{A}^m$  of any even order  $m$  contains the tensor  $\mathbf{A}^{m+2}$ . In order to

resolve this dilemma, it is customary to approximate  $\mathcal{A}$  by a so-called closure approximation, in terms of  $\mathbf{A}$ .

Many examples of closure approximations can be found in [1, 37]. The simplest are the linear and quadratic approximations, denoted by  $\mathcal{A}^L$  and  $\mathcal{A}^Q$ , respectively.

The linear closure is defined by

$$\mathcal{A}^L \mathbf{D} = -\frac{1}{35} ((\text{tr } \mathbf{D}) \mathbf{I} + 2\mathbf{D}) + \frac{1}{7} [(\text{tr } \mathbf{D}) \mathbf{A} + 2\mathbf{A}\mathbf{D} + 2\mathbf{D}\mathbf{A} + (\mathbf{A} : \mathbf{D}) \mathbf{I}] \quad (2.37)$$

In the case that we want to consider, the fluid is incompressible, so

$$\text{tr } \mathbf{D} = 0. \quad (2.38)$$

Then (2.37) becomes

$$\mathcal{A}^L \mathbf{D} = -\frac{2}{35} \mathbf{D} + \frac{1}{7} [2\mathbf{A}\mathbf{D} + 2\mathbf{D}\mathbf{A} + (\mathbf{A} : \mathbf{D}) \mathbf{I}]. \quad (2.39)$$

The linear approximation is exact for random orientations, in which case

$$\mathbf{A} = \begin{pmatrix} 1/n & 0 & \dots & 0 \\ 0 & 1/n & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & \dots & 0 & 1/n \end{pmatrix}$$

for a problem in  $\mathbb{R}^n$  (see [37]).

The quadratic closure is defined by

$$\mathcal{A}_{ijkl}^Q = A_{ij} A_{kl}. \quad (2.40)$$

The quadratic closure approximation is exact for any unidirectional state, e.g.

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

in which the fibres are aligned with the  $x_1$ -axis of the coordinate system chosen (see [37]).

The above two approximations are reasonable approximations in particular flow situations. Hinch and Leal [2, 8] have developed two alternative closure rules, commonly denoted by H&L1 and H&L2. These closures give good results for low intermediate alignment, but the rule H&L2 displays artificial oscillations in simple shear flow.

Advani and Tucker tried to maximise the accuracy of the linear and quadratic rules by defining the hybrid closure approximation [2], which is a combination of these two closures. They showed that this new closure generally leads to good approximations, when compared with results obtained by solving the equations for  $\psi$  and  $\mathbf{p}$  directly.

The hybrid closure is defined by

$$\mathcal{A}^H = (1 - f)\mathcal{A}^L + f\mathcal{A}^Q, \quad (2.41)$$

for  $0 \leq f \leq 1$ ;  $f$  is in general a function of  $\mathbf{A}$ , and the hybrid approximation is therefore not a linear combination of the linear and the quadratic approximations.

Advani and Tucker have proposed the use of [2, 37]

$$f(\mathbf{A}) = 1 - N \det \mathbf{A}, \quad (2.42)$$



where  $N$  equals 4 for a planar flow and 27 for fully three-dimensional situations. An alternative proposal is [1]

$$f(\mathbf{A}) = a|\mathbf{A}|^2 - b, \quad (2.43)$$

where  $(a, b) = (2, 1)$  and  $(\frac{3}{2}, \frac{1}{2})$  in two and three dimensions, respectively.

Recently, Cintra and Tucker ([8]) have developed a new family of orthotropic closures. These new closures are based on the fundamental observation that the tensor  $\mathcal{A}$  must be orthotropic. Two closure rules are studied in detail: the smooth closure and the fitted closure. The former has a simple form based on linear interpolation of the eigenvalues of  $\mathbf{A}$ , while the fitted closure is based on numerical solutions for the probability density functions.

### 2.2.3 Constitutive equation for the stress

For fibre suspensions, the stress tensor  $\mathbf{T}$  is given by [37]

$$\mathbf{T} = -p\mathbf{I} + 2\mu\mathbf{D} + \mathcal{T}^E, \quad (2.44)$$

where  $p$  is the pressure,  $\mu$  the solvent viscosity and  $\mathcal{T}^E$  the extra stress tensor, which is given by

$$\mathcal{T}^E = 2\mu c (E\mathbf{A}\mathbf{D} + B(\mathbf{D}\mathbf{A} + \mathbf{A}\mathbf{D}) + C\mathbf{D} + 2F\mathbf{D}_r\mathbf{A}). \quad (2.45)$$

Here  $c$  is the particle volume fraction and  $E$ ,  $B$ ,  $C$  and  $F$  are positive

material constants. The term  $D_r$  accounts for Brownian motion; it is significant when particles are near molecular size, but is negligible for larger fibres, such as those that are found in reinforced polymers [37]. Using the case of slender body theory [1, 2, 37] and assuming that  $D_r = 0$ , equation (2.45) can be written as

$$\mathcal{T}^E = 2\mu c (EAD + B(DA + AD) + CD) . \quad (2.46)$$

Inserting equation (2.46) in equation (2.44), we find that

$$\begin{aligned} \mathbf{T} &= -p\mathbf{I} + 2\mu\mathbf{D} + 2\mu c (EAD + B(DA + AD) + CD) \\ &= -p\mathbf{I} + 2\mu\mathbf{D}(1 + cC) + 2\mu c (EAD + B(DA + AD)) \\ &= -p\mathbf{I} + 2\mu\mathbf{D}(1 + cC) \\ &\quad + 2\mu \frac{c}{1 + cC} (EAD + B(DA + AD)) (1 + cC) \\ &= -p\mathbf{I} + 2\mu(1 + cC)\mathbf{D} \\ &\quad + 2\mu(1 + cC) \left( \frac{cE}{1 + cC} AD + \frac{cB}{1 + cC} (DA + AD) \right) \\ &= -p\mathbf{I} + 2\mu_I \mathbf{D} + \mathbf{S}, \end{aligned} \quad (2.47)$$

in which

$$\mathbf{S} = 2\mu_I (N_p AD + N_s (DA + AD)) , \quad (2.48)$$

$$\mu_I = \mu(1 + cC) , \quad (2.49)$$

$$N_p = \frac{cE}{1 + cC} , \quad (2.50)$$

$$N_s = \frac{cB}{1 + cC} . \quad (2.51)$$

The positive constants  $N_p$  and  $N_s$  are called respectively, the particle number and shear number.

$A(x, t)$ , which satisfy the following set of equations:

*conservation of linear momentum*

$$\rho \frac{\partial v}{\partial t} + (v \cdot \nabla) v - \operatorname{div} T = \rho b; \quad (2.56)$$

*conservation of mass (continuity equation)*

$$\operatorname{div} v = 0; \quad (2.57)$$

*constitutive equation for the stress*

$$T = -pI + 2\mu_I (D + N_p AD + N_s(DA + AD)); \quad (2.58)$$

*the evolution equation for the orientation tensor*

$$\frac{DA}{Dt} + AW - WA - \lambda(DA + AD - 2AD) - D_r(I - nA) = 0; \quad (2.59)$$

*the boundary conditions*

$$v = \bar{v} \text{ on } \Gamma_v \text{ and } Tn = \bar{t} \text{ on } \Gamma_t;$$

*and the initial conditions*

$$v(x, 0) = v_0, \quad A(x, 0) = A_0 \text{ on } \bar{\Omega}. \quad (2.60)$$

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## Chapter 3

# Thermodynamical analysis

In this chapter we investigate the conditions under which the constitutive equations for fibre suspensions, as presented in Chapter 2, are consistent with the second law of thermodynamics. This law, which in the present context takes the form of the Clausius-Duhem inequality or reduced dissipation inequality, is used to identify conditions which the constitutive equations have to satisfy. We also investigate in this chapter the question of stability of fibre suspension flows, by examining the behaviour of the kinetic energy of the system with time. The study is restricted to the linear and quadratic closures.

In Section 3.1 various preliminary notions are discussed. These lead to a statement of the second law in a form that is appropriate for this study. Restrictions on the constitutive equations are investigated in Section 3.2, and stability is the subject of Section 3.3.

## 3.1 Continuum thermodynamics

### 3.1.1 Internal state variables

In this section, we will review the thermodynamics of materials with internal state variables, [9, 10]. The materials which are considered here are those whose behaviour can be described through the stress tensor  $\mathbf{T}$ , the heat flux vector  $\mathbf{q}$ , the specific Helmholtz free energy  $\psi$ , and the specific entropy  $\eta$ . The state or dependent variables are: the temperature  $\theta$ , the deformation gradient  $\mathbf{F}$ , the temperature gradient  $\mathbf{g}$ , and a set of  $N$  internal or “hidden” state variables, which in the present context is the orientation tensor  $\mathbf{A}$ . The rate of change of the internal variable must be specified by an evolution equation as a function of some or all of the state variables, including the internal variable itself.

Consider a body  $\mathcal{B}$  with an arbitrary material point denoted by  $\mathbf{X}$ , and assume that the mechanical forces acting on  $\mathcal{B}$  can always be resorbed into a body force field and a symmetric stress field. It is assumed that  $\mathcal{B}$  may deform and conduct heat. The state of the body is described by nine functions of  $\mathbf{X}$  and time  $t$ , as follows [9, 10]:

- (1) The motion  $\mathbf{x} = \chi(\mathbf{X}, t)$ , where  $\mathbf{x}$  denotes spatial position;
- (2) The symmetric Cauchy stress tensor  $\mathbf{T} = \mathbf{T}(\mathbf{X}, t)$  ;
- (3) The specific body force  $\mathbf{b} = \mathbf{b}(\mathbf{X}, t)$  per unit mass (exerted on  $\mathcal{B}$  at the external world, i.e., by other bodies which do not intersect  $\mathcal{B}$ );
- (4) The specific internal energy  $\varepsilon = \varepsilon(\mathbf{X}, t)$  per unit mass;
- (5) The heat flux vector  $\mathbf{q} = \mathbf{q}(\mathbf{X}, t)$  ;
- (6) The heat supply  $r = r(\mathbf{X}, t)$  per unit mass and unit time (absorbed by  $\mathcal{B}$  at  $\mathbf{X}$  and furnished by the external world );

- (7) The specific entropy  $\eta = \eta(\mathbf{X}, t)$  per unit mass;
- (8) The absolute temperature  $\theta = \theta(\mathbf{X}, t) > 0$ ; and
- (9) The internal variable  $\mathbf{A} = \mathbf{A}(\mathbf{X}, t)$ .

The set of nine functions above defined for all  $\mathbf{X}$  in  $\mathcal{B}$  is called a *thermodynamic process in  $\mathcal{B}$*  if and only if it is compatible with the laws of balance of linear momentum and of energy [9, 10].

Denote by  $\mathbf{L}$  the velocity gradient: that is,

$$\mathbf{L} \equiv \nabla \mathbf{v} \quad \text{or} \quad L_{ij} = \frac{\partial v_i}{\partial x_j}.$$

**Law of balance of energy.** This is given in local form by [9]

$$\rho \dot{\epsilon} - \mathbf{T} : \mathbf{L} + \operatorname{div} \mathbf{q} = \rho r. \quad (3.1)$$

**Entropy production**[9]. The specific rate  $\gamma$  of production of entropy is defined by

$$\gamma = \dot{\eta} - \left[ \left( \frac{r}{\theta} - \frac{1}{\rho} \operatorname{div} \left( \frac{\mathbf{q}}{\theta} \right) \right) \right], \quad (3.2)$$

in which  $\mathbf{q}/\theta$  is a flux of entropy (due to the heat flow) and  $r/\theta$  is the supply of entropy due to radiation.

**Theorem 3.1** *The specific rate of entropy production may be expressed in the form*

$$\gamma = \dot{\eta} - \frac{\dot{\epsilon}}{\theta} + (\rho\theta)^{-1} \mathbf{T} : \mathbf{L} - \frac{1}{\rho\theta^2} \mathbf{q} \cdot \mathbf{g}. \quad (3.3)$$

**Proof.** After multiplying (3.2) by  $\rho$  and substituting (3.1) in (3.2) we have

$$\rho\gamma = \rho\dot{\eta} - \left[ \rho \frac{\dot{\epsilon}}{\theta} - \frac{1}{\theta} \mathbf{T} : \mathbf{L} + \frac{\operatorname{div} \mathbf{q}}{\theta} - \operatorname{div} \left( \frac{\mathbf{q}}{\theta} \right) \right]. \quad (3.4)$$

That is,

$$\gamma = \dot{\eta} - \frac{\dot{\varepsilon}}{\theta} + \left( \frac{1}{\rho\theta} \right) \mathbf{T} : \mathbf{L} - \frac{1}{\rho} \left( \frac{\operatorname{div} \mathbf{q}}{\theta} - \operatorname{div} \left( \frac{\mathbf{q}}{\theta} \right) \right). \quad (3.5)$$

The fourth term of (3.5) on the right hand side is equal to

$$\begin{aligned} \frac{\operatorname{div} \mathbf{q}}{\theta} - \operatorname{div} \left( \frac{\mathbf{q}}{\theta} \right) &= \frac{q_{i,i}}{\theta} - \frac{q_{i,i}\theta - q_i\theta_{,i}}{\theta^2} \\ &= \frac{q_i}{\theta^2} \theta_{,i} \\ &= \frac{1}{\theta^2} \mathbf{q} \cdot \mathbf{g}. \end{aligned} \quad (3.6)$$

Hence, substitution of (3.6) in (3.5) gives

$$\gamma = \dot{\eta} - \frac{\dot{\varepsilon}}{\theta} + (\rho\theta)^{-1} \mathbf{T} : \mathbf{L} - \frac{1}{\rho\theta^2} \mathbf{q} \cdot \mathbf{g}. \quad (3.7)$$

In what follows, it is more convenient to make use of the *free energy*  $\psi$ , rather than the internal energy  $\varepsilon$ . The free energy is related to the internal energy by [9]

$$\psi = \varepsilon - \theta\eta. \quad (3.8)$$

It follows that

$$\dot{\psi} = \dot{\varepsilon} - \dot{\theta}\eta - \dot{\eta}\theta, \quad (3.9)$$

so that (3.7) now becomes

$$\theta\gamma = -\dot{\psi} - \dot{\theta}\eta + \frac{1}{\rho} \mathbf{T} : \mathbf{L} - (\rho\theta)^{-1} \mathbf{q} \cdot \mathbf{g}. \quad (3.10)$$

**The Clausius–Duhem inequality.** The second law of thermodynamics may be expressed in the form of the Clausius–Duhem inequality, which asserts that

$$\gamma \geq 0 \quad (3.11)$$



for all admissible processes.

We will be concerned only with *isothermal processes*, for which  $\theta$  is constant and  $\mathbf{g} = \mathbf{0}$ . For such processes the Clausius-Duhem inequality becomes the *dissipation inequality*

$$\rho \dot{\psi} \leq \mathbf{T} : \mathbf{L}. \quad (3.12)$$

This inequality will form the basis of our investigation of the constitutive equations for fibre suspensions. It states that, in an isothermal process, the rate of increase in the free energy of a system may not exceed the rate of work.

### 3.2 Constitutive equations

In an isothermal process, the behaviour of a material point  $\mathbf{X}$  is characterised by

- (a) two response functions, viz. the free energy and stress, which are generally functions of the deformation and the internal variable;
- (b) an equation which describes the evolution of the internal variable.

In the present context the internal variable is the orientation tensor  $\mathbf{A}$ . In addition, we are dealing with incompressible flows, for which the stress is determined only up to a hydrostatic pressure. Thus the full set of constitutive equations takes the form

$$\psi = \hat{\psi}(\mathbf{F}, \mathbf{A}), \quad (3.13)$$

$$\mathbf{T} = -p\mathbf{I} + \hat{\mathbf{T}}(\mathbf{L}, \mathbf{A}), \quad (3.14)$$

$$\dot{\mathbf{A}} = \hat{\mathbf{f}}(\mathbf{L}, \mathbf{A}). \quad (3.15)$$

For fibre suspensions the constitutive equation for the stress is given by (2.47); that is,

$$\mathbf{T} = -p\mathbf{I} + 2\mu\mathbf{D} + \mathbf{S}. \quad (3.16)$$

The evolution equation (3.15) is given by (2.36); that is,

$$\dot{\mathbf{A}} = (\mathbf{W}\mathbf{A} - \mathbf{A}\mathbf{W}) + \lambda(\mathbf{D}\mathbf{A} + \mathbf{A}\mathbf{D} - 2\mathcal{A}\mathbf{D}) + 2\sqrt{2}C_I|\mathbf{D}|(\mathbf{I} - n\mathbf{A}). \quad (3.17)$$

Making use of (3.14) and (3.15) in the dissipation inequality (3.12), we find that

$$\rho\psi_{\mathbf{F}} : \dot{\mathbf{F}} + \rho\psi_{\mathbf{A}} : \dot{\mathbf{A}} + p\mathbf{I} : \mathbf{L} - \widehat{\mathbf{T}} : \mathbf{L} \leq 0, \quad (3.18)$$

since

$$\dot{\psi}(\mathbf{F}, \mathbf{A}) = \psi_{\mathbf{F}} : \dot{\mathbf{F}} + \psi_{\mathbf{A}} : \dot{\mathbf{A}} \quad (3.19)$$

and  $\psi_{\mathbf{F}}$  and  $\psi_{\mathbf{A}}$  are respectively the derivatives of  $\psi$  with respect to  $\mathbf{F}$  and  $\mathbf{A}$ .

The inverse of  $\mathbf{F}$  exists, and the velocity gradient is related to  $\dot{\mathbf{F}}$  by

$$\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1}, \quad (3.20)$$

(see for example, [9, 10]).

Next, we substitute (3.16) and (3.17) in (3.18), and use of (3.20) and also the fact that  $\mathbf{I} : \mathbf{L} = 0$  from the incompressibility assumption, to get

$$\begin{aligned} \rho\psi_{\mathbf{F}}\mathbf{F}^T : \mathbf{L} &+ \rho\psi_{\mathbf{A}} : \left[ \mathbf{A}\mathbf{W} - \mathbf{W}\mathbf{A} - \lambda(\mathbf{A}\mathbf{D} + \mathbf{D}\mathbf{A} - 2\mathcal{A}\mathbf{D}) \right] \\ &+ \rho\psi_{\mathbf{A}} : 2\sqrt{2}C_I|\mathbf{D}|(\mathbf{I} - n\mathbf{A}) \\ &- \left[ 2\mu_I\mathbf{D} + 2\mu_I(N_p\mathcal{A}\mathbf{D} + N_s(\mathbf{D}\mathbf{A} + \mathbf{A}\mathbf{D})) \right] : \mathbf{L} \leq 0. \end{aligned} \quad (3.21)$$

Since  $\mathbf{L}$  is arbitrary, we may replace it by  $\alpha \mathbf{L}$  ( $\alpha \in \mathbb{R}$ ) in (3.21) and using the symmetry of the stress  $\mathbf{T}$  to obtain

$$\alpha \left[ G - (\operatorname{sgn} \alpha) M \right] - \alpha^2 K \leq 0, \quad (3.22)$$

in which

$$\begin{aligned} \rho^{-1} G &= \psi_{\mathbf{F}} \mathbf{F}^T : \mathbf{L} + \psi_{\mathbf{A}} : \left[ \mathbf{A} \mathbf{W} - \mathbf{W} \mathbf{A} - \lambda (\mathbf{D} \mathbf{A} + \mathbf{A} \mathbf{D} - 2 \mathbf{A} \mathbf{D}) \right], \\ M &= \rho 2 \sqrt{2} C_I |\mathbf{D}| \psi_{\mathbf{A}} : (\mathbf{I} - n \mathbf{A}), \end{aligned} \quad (3.23)$$

$$K = \left[ 2 \mu_I \mathbf{D} + 2 \mu_I (N_p \mathbf{A} \mathbf{D} + N_s (\mathbf{D} \mathbf{A} + \mathbf{A} \mathbf{D})) \right] : \mathbf{D} \quad (3.24)$$

$$= \mathbf{T}(\mathbf{D}, \mathbf{A}) : \mathbf{D} \quad (3.25)$$

and

$$\operatorname{sgn} \alpha = \begin{cases} +1 & \text{for } \alpha \geq 0 \\ -1 & \text{for } \alpha < 0 \end{cases}$$

**Proposition 3.1** *Equation (3.22) holds if and only if*

$$\begin{aligned} M &\geq 0, \\ K &\geq 0, \\ G &\leq |M|. \end{aligned} \quad (3.26)$$

**Proof.**

1. Suppose that  $\alpha = 0$ : then (3.22) holds.
2. Suppose that  $\alpha > 0$ : then (3.22) becomes

$$G - M - \alpha K \leq 0. \quad (3.27)$$

Thus (3.27) holds if and only if

$$G - M \leq 0 \quad (3.28)$$

and

$$K \geq 0, \quad (3.29)$$

because  $\alpha$  is positive and may be chosen to be arbitrary small.

3. Let us suppose next that  $\alpha < 0$ : then (3.22) can be written as,

$$(G + M) + |\alpha|K \geq 0. \quad (3.30)$$

Therefore we deduce that

$$G + M \geq 0 \quad (3.31)$$

and

$$K \geq 0. \quad (3.32)$$

Finally, equations (3.28) and (3.31) hold if and only if  $G \leq |M|$ . It follows that since  $\rho \geq 0$ , then  $K \geq 0$ ,  $M \geq 0$  and  $G \leq |M|$ .  $\square$

$K \geq 0$  implies that

$$\left[ 2\mu_I \mathbf{D} + 2\mu_I (N_p \mathcal{A} \mathbf{D} + N_s (\mathbf{D} \mathbf{A} + \mathbf{A} \mathbf{D})) \right] : \mathbf{D} \geq 0; \quad (3.33)$$

this inequality is used to determine restrictions on the constitutive equations for the stress **Linear closure approximation**. By substituting  $\mathcal{A}^L \mathbf{D}$  by the equation (2.39) in (3.33), we have

$$\begin{aligned} K &= 2\mu_I \left[ \mathbf{D} - \frac{2}{35} N_p \mathbf{D} + \frac{1}{7} N_p (2\mathbf{A} \mathbf{D} + 2\mathbf{D} \mathbf{A}) + N_s (\mathbf{D} \mathbf{A} + \mathbf{A} \mathbf{D}) \right] : \mathbf{D} \\ &= 2\mu_I \left[ \left( 1 - \frac{2}{35} N_p \right) \mathbf{D} : \mathbf{D} + \frac{2}{7} N_p (\mathbf{A} \mathbf{D} + \mathbf{D} \mathbf{A}) : \mathbf{D} \right] \\ &\quad + 2\mu_I [N_s (\mathbf{D} \mathbf{A} + \mathbf{A} \mathbf{D}) : \mathbf{D}] \end{aligned}$$

$$\begin{aligned}
&= 2\mu_I \left[ \left(1 - \frac{2}{35}N_p\right) |D|^2 + \frac{2}{7}N_p(AD + DA) : D \right] \\
&+ 2\mu_I \left[ N_s(DA + AD) : D \right] \\
&= 2\mu_I \left[ \left(1 - \frac{2}{35}N_p\right) |D|^2 + \frac{2}{7}N(A : D^2) \right] \geq 0, \tag{3.34}
\end{aligned}$$

using the Corollary A.2 (see the Appendix) and substituting  $N$  by  $2N_p + 7N_s$ .

(3.34) implies that

$$7 \left(1 - \frac{2}{35}N_p\right) |D|^2 + N(A : D^2) \geq 0, \tag{3.35}$$

since  $\mu_I > 0$ . The inequality (3.35) holds if  $\left(1 - \frac{2}{35}N_p\right) \geq 0$ , because  $A : D^2 = \sum_{i=1}^n A_{ii} D_{ii}^2 \geq 0$  (since  $A$  is positive by definition).

So the inequality 3.35 holds for

$$N_p \leq \frac{35}{2} \tag{3.36}$$

and for all flows.

**Theorem 3.2** *The constitutive equations (2.58) and (2.59) with the linear closure approximation (2.37) are compatible with the second law of thermodynamics if and only if*

$$N_p \leq \frac{35}{2} \tag{3.37}$$

**Quadratic closure approximation.** By using the proposition 3.1, we have

$$|D|^2 + N_p(A : D)^2 + 2N_s A : D^2 \geq 0. \tag{3.38}$$

One can see (3.38) holds for any flow field and orientation tensor field.

**Theorem 3.3** *The constitutive equations (2.58) and (2.59) with the quadratic closure approximation (2.40) are compatible with the second law of thermodynamics.*

### 3.3 Energetic stability

We consider (2.10). Next, we form the scalar product of (2.9) with  $\mathbf{v}$ , integrate over the domain  $\Omega$  and using the divergence theorem and the law of conservation of mass to get

$$\frac{1}{2} \frac{d}{dt} \int_{\Omega} \rho |\mathbf{v}|^2 dx + \int_{\Omega} \mathbf{T} : \mathbf{L} dx = \int_{\Gamma} \mathbf{v} \cdot \mathbf{T} \mathbf{n} ds + \int_{\Omega} \rho \mathbf{v} \cdot \mathbf{b} dx \quad (3.39)$$

in which  $\mathbf{n}$  is the unit outward normal to  $\Gamma$ .

We assume that the body is mechanically isolated [11], so that

$$\int_{\Gamma} \mathbf{v} \cdot \mathbf{T} \mathbf{n} ds + \int_{\Omega} \rho \mathbf{v} \cdot \mathbf{b} dx = 0, \quad (3.40)$$

so that (3.39) becomes

$$\frac{1}{2} \frac{d}{dt} \int_{\Omega} \rho |\mathbf{v}|^2 dx + \int_{\Omega} \mathbf{T} : \mathbf{L} dx = 0. \quad (3.41)$$

We denote by  $E$  the kinetic energy of the fluid; that is,

$$E(t) = \frac{1}{2} \int_{\Omega} \rho |\mathbf{v}|^2 dx; \quad (3.42)$$

then (3.41) becomes

$$E'(t) = - \int_{\Omega} \mathbf{T} : \mathbf{L} dx. \quad (3.43)$$

Our interest is first to determine the conditions under which fibre suspension flows are monotonically stable, for linear and quadratic closures, in the sense that

$$E'(t) \leq 0 \text{ for all } t. \quad (3.44)$$

Substitution of (2.47) and (2.48) in (3.43) leads to the equation

$$E'(t) = -2\mu_I |D|^2 - 2\mu_I \int_{\Omega} (N_s A : D^2 + N_p A D : D) \, dx. \quad (3.45)$$

**Case of linear closure.** Substitution of (2.39) in (3.45) and the use of the incompressibility property give as earlier give

$$E'(t) = -\frac{4\mu_I N}{7} \int_{\Omega} A : D^2 \, dx - 2\mu_I \left(1 - \frac{2}{35} N_p\right) |D|^2, \quad (3.46)$$

for the rate of change of kinetic energy.

For all  $t > 0$ , and for all admissible fields  $v$  and  $A$ , we see from (3.46) and from the positivity of  $A : D^2$  that (3.44) holds in the event that  $N_p \leq 35/2$ . Thus we conclude that approximations with the linear closure are monotonically stable if  $N_p \leq 35/2$ .

Furthermore, from the inequalities of Korn and Poincaré-Friedrichs (see theorem B.2, in the Appendix B), there exists a constant  $c_1 > 0$  such that

$$|D|^2 \geq c_1 E(t); \quad (3.47)$$

thus, from (3.46) we have

$$\begin{aligned} E'(t) + \lambda E(t) &\leq E'(t) + \frac{2}{\rho} \mu_I \left(1 - \frac{2}{35} N_p\right) \|D\|^2 \\ &= -\frac{4}{7} \frac{\mu_I}{\rho} N \int_{\Omega} A : D^2 \, dx \\ &\leq 0, \end{aligned} \quad (3.48)$$

where  $\lambda = \frac{2c_1\mu_I}{\rho} \left(1 - \frac{2N_p}{35}\right) > 0$ . It follows, by integration of (3.48), that

$$E(t) \leq E(0)e^{-\lambda t} \text{ for all } t, \quad (3.49)$$

which means that the approximations with linear closure are exponentially stable if  $N_p \leq \frac{35}{2}$ .

**Theorem 3.4** *Assume that inequality (3.36) holds. Then the fibre suspension flows corresponding to the linear closure approximation are stable. Furthermore, the energy increases exponentially.*

**Case of quadratic closure.** By inserting the equations (2.40) in the equation (3.45) we have

$$E'(t) = - \left[ 2\mu_I |D|^2 + 2\mu_I N_p \int_{\Omega} (A : D)^2 dx + 4\mu_I N_s \int_{\Omega} A : D^2 dx \right]. \quad (3.50)$$

Since  $A : D^2$  (because  $A$  is positive defined) and all the terms are nonnegative as well, we have that  $E'(t) \leq 0$  for all  $t \geq 0$ . This implies that there is a monotonic stability for the case of quadratic closure.

(3.50) can be written as follows

$$E'(t) + 2\mu_I |D|^2 = -2\mu_I \left( N_p \int_{\Omega} (A : D)^2 dx + 2N_s \int_{\Omega} A : D^2 dx \right) \leq 0, \quad (3.51)$$

as previously, by application of the inequalities of Korn and Poincaré-Friedrichs, we have exponential stability for quadratic closure.

**Theorem 3.5** *Fibre suspension flows with the quadratic closure are stable.*



# Chapter 4

## One-dimensional problem

This chapter is about some very specific problems involving fibre suspensions. We specialise the general theory of fibre suspensions to the particular cases of unidirectional flow, and find the exact solution for the former case.

### 4.1 Unidirectional problem

Consider the unidirectional flow  $\mathbf{v} = u(x)\mathbf{e}_1$ . For this flow,

$$\mathbf{L} = \begin{pmatrix} \frac{du}{dx} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \mathbf{D} \quad (4.1)$$

and  $\mathbf{W} = \mathbf{0}$ .

The incompressibility condition  $\text{div} \mathbf{v} = 0$  implies that  $\frac{du}{dx} = 0$ , so that we must have  $u = \text{constant}$ . From (4.1), therefore, we see that  $\mathbf{D} = \mathbf{0}$ ,

and for this very simple flow, (2.36) becomes

$$\dot{\mathbf{A}} - D_r(\mathbf{I} - 3\mathbf{A}) = \mathbf{0}. \quad (4.2)$$

The fact that  $\mathcal{A}$  does not appear in (4.2) means that the orientation is independent of closure approximation.

Since the flow is steady, (4.2) is equivalent to

$$u \frac{d\mathbf{A}}{dx} + 3D_r\mathbf{A} = D_r\mathbf{I}, \quad (4.3)$$

or

$$\frac{u}{D_r} \frac{d\mathbf{A}}{dx} + 3\mathbf{A} = \mathbf{I}. \quad (4.4)$$

By setting

$$\frac{u}{D_r} = \gamma$$

(4.4) becomes

$$\gamma \frac{d\mathbf{A}}{dx} + 3\mathbf{A} = \mathbf{I}. \quad (4.5)$$

As one can see, (4.5) is analogous to the problem in [34], with  $\gamma$  here playing the role of Weissenberg number.

## 4.2 Exact solution

Dividing throughout by  $\gamma$  and multiplying (4.5) by  $\exp\left(\frac{3x}{\gamma}\right)$ , we have

$$\exp\left(\frac{3x}{\gamma}\right) \left( \frac{d\mathbf{A}}{dx} + 3\frac{\mathbf{A}}{\gamma} \right) = \exp\left(\frac{3x}{\gamma}\right) \frac{\mathbf{I}}{\gamma}. \quad (4.6)$$

Note that

$$\begin{aligned}\frac{d}{dx} \left( \exp \left( \frac{3x}{\gamma} \right) \mathbf{A} \right) &= \exp \left( \frac{3x}{\gamma} \right) \frac{d\mathbf{A}}{dx} + \frac{3}{\gamma} \exp \left( \frac{3x}{\gamma} \right) \mathbf{A} \\ &= \exp \left( \frac{3x}{\gamma} \right) \left( \frac{d\mathbf{A}}{dx} + 3 \frac{\mathbf{A}}{\gamma} \right)\end{aligned}\quad (4.7)$$

By identification of equations (4.6) and (4.7), we have

$$\frac{d}{dx} \left( \exp \left( \frac{3x}{\gamma} \right) \mathbf{A} \right) = \exp \left( \frac{3x}{\gamma} \right) \frac{\mathbf{I}}{\gamma} \quad (4.8)$$

So that, after integration,

$$\exp \left( \frac{3x}{\gamma} \right) \mathbf{A} = \int_0^x \exp \left( \frac{3\tau}{\gamma} \right) \frac{\mathbf{I}}{\gamma} d\tau \quad (4.9)$$

The solution of (4.5) is thus

$$\mathbf{A} = \frac{\exp \left( \frac{-3x}{\gamma} \right)}{\gamma} \mathbf{I} \int_0^x \exp \left( \frac{3\tau}{\gamma} \right) d\tau \quad (4.10)$$

or, in index form,

$$A_{ij} = \frac{\exp \left( \frac{-3x}{\gamma} \right)}{\gamma} \delta_{ij} \int_0^x \exp \left( \frac{3\tau}{\gamma} \right) d\tau. \quad (4.11)$$

### 4.3 Study of the exact solution

As  $\gamma \rightarrow \infty$ ,  $A_{ij} \rightarrow 0$ , and the constraint  $A_{ii} = 1$  is not satisfied. To circumvent this problem we set  $\mathbf{A} = \tilde{\mathbf{A}} + \mathbf{A}^*$ , where  $\mathbf{A}^*$  is constant tensor with  $\mathbf{A}_{ii}^* = 1$ .

Then (4.5) becomes

$$\gamma \frac{d\tilde{\mathbf{A}}}{dx} + 3\tilde{\mathbf{A}} = \mathbf{f}, \quad (4.12)$$

in which  $f = I - 3A^*$ , a constant.

As previously, one can see that the exact solution of (4.12) is

$$\tilde{A} = \frac{\exp\left(\frac{-3x}{\gamma}\right)}{\gamma} f \int_0^x \exp\left(\frac{3\tau}{\gamma}\right) d\tau, \quad (4.13)$$

and we see that as  $\gamma \rightarrow \infty$ ,  $\tilde{A} \rightarrow 0$ . Thus we conclude that for high  $\gamma$ , where  $\tilde{A}$  is small, the equation (4.12) can be approximated by

$$\gamma \frac{d\tilde{A}}{dx} \approx f. \quad (4.14)$$

## Chapter 5

# Finite element approximations

The first section of this chapter will be a review of the finite element method (Galerkin method, Streamline Upwind (SU) and Streamline Upwind Petrov/Galerkin (SUPG)), which we will apply to a model one-dimensional problem. In the first section of this chapter, we define the abstract continuous problem, of which the unidirectional flow equation is a special case. The second section of this chapter will be taken up with a review of the finite element method. Then we will apply the finite element method to the given problem of Section 5.1. The Galerkin approximation does not lead to good approximations in the case where a convective term dominates, and when the exact solution is not sufficiently smooth [24]. Thus we will use the Streamline Upwind (SU) and Streamline Upwind Petrov/Galerkin (SUPG) methods, and show that finite element approximations converge for these two methods. In the third section of this chapter, we apply the general theory to the problem of unidirectional flow of fibre suspensions.

## 5.1 The continuous problem

Here we follow the treatment in [24]. We consider the problem

$$\begin{cases} \frac{\partial u}{\partial t} + \beta \frac{du}{dx} + \sigma u = f & \text{in } \Omega \times I, \\ u(a) = g, \end{cases}$$

where  $\beta$  is a constant, positive velocity field,  $\sigma$  an absorption coefficient,  $u$  a scalar unknown representing a concentration, for example,  $f$  is a source function,  $I$  a given time interval,  $\Omega = (a, b)$  is the domain, an interval on the real line, and  $\Gamma = \{a, b\}$  is the boundary of  $\Omega$ .

The steady version of this problem is of interest here, so we consider the problem

$$\begin{cases} \beta \frac{du}{dx} + u = f & \text{in } \Omega, \\ u(a) = g, \end{cases} \quad (5.1)$$

where for convenience we have also set  $\sigma = 1$ .

**Remark 5.1** The exact solution of (5.1) is

$$u = \frac{\exp\left(\frac{-x}{\beta}\right)}{\beta} \int_a^x f(y) \exp\left(\frac{y}{\beta}\right) dy. \quad (5.2)$$

From (5.2),  $u \rightarrow 0$  as  $\beta \rightarrow \infty$ . For large  $\beta$ , we may therefore approximate (5.1) by

$$\beta \frac{du}{dx} \approx f. \quad (5.3)$$

### 5.1.1 Finite element approximations

We partition  $\Omega = (a, b)$  according to  $x_0 = a < x_1 < x_2 < \dots < x_N = b$ , and define the finite element  $\Omega_i = (x_{i-1}, x_i)$  of length  $h_i$ , for  $i = 1, \dots, N$ . The mesh parameter  $h$  is defined by

$$h = \max_i h_i \quad (1 \leq i \leq N). \quad (5.4)$$

#### Function spaces and notation

We will require the Sobolev space

$$H^1(\Omega) = \left\{ u \in L^2(\Omega) : \frac{du}{dx} \in L^2(\Omega) \right\}, \quad (5.5)$$

where  $L^2(\Omega)$  is the space of square integrable functions on  $\Omega$ ; see the definition (B.6) in Appendix B.

More generally, we introduce the Sobolev space

$$H^s(\Omega) = \left\{ v \in L^2(\Omega) : \frac{d^\alpha v}{dx^\alpha} \in L^2(\Omega), \alpha = 0, \dots, s \right\} \quad (5.6)$$

for nonnegative integer  $s$ ; this is a Hilbert space with inner product and norm defined by

$$(u, v) = \int_a^b \sum_{\alpha=0}^s \frac{d^\alpha u}{dx^\alpha} \frac{d^\alpha v}{dx^\alpha} dx, \quad (5.7)$$

$$\|v\|_s \equiv \|v\|_{H^s(\Omega)} = \left( \int_a^b \sum_{\alpha=0}^s \left( \frac{d^\alpha v}{dx^\alpha} \right)^2 dx \right)^{\frac{1}{2}}. \quad (5.8)$$

For the case  $s = 0$  we write

$$\|u\|_0 \equiv \|u\|.$$

The seminorm on  $H^s(\Omega)$  is defined by

$$|v|_s \equiv |v|_{H^s(\Omega)} = \left( \int_a^b \sum_{\alpha=s} \left( \frac{d^\alpha v}{dx^\alpha} \right)^2 dx \right)^{\frac{1}{2}}. \quad (5.9)$$

We also use the notation

$$\langle v, w \rangle = \left[ \beta v w \right]_a^b = (\beta v w)(b) - (\beta v w)(a), \quad (5.10)$$

$$\langle v, w \rangle_- = (\beta v w)(a), \quad (5.11)$$

$$\langle v, w \rangle_+ = (\beta v w)(b), \quad (5.12)$$

and

$$|v| = \langle v, v \rangle^{\frac{1}{2}}. \quad (5.13)$$

We also note that

$$\langle v, v \rangle = \langle v, v \rangle_+ + \langle v, v \rangle_-. \quad (5.14)$$

Next we define the finite element space  $V_h$  according to

$$V_h = \{v \in H^1(\Omega) : v|_{\Omega_i} \in P_1(\Omega_i), \text{ for all finite elements } \Omega_i\}, \quad (5.15)$$

in which  $P_1$  is the space of polynomials of degree not exceeding 1 on  $\Omega_i$ .

Note that  $V_h \subset C(\bar{\Omega})$ .



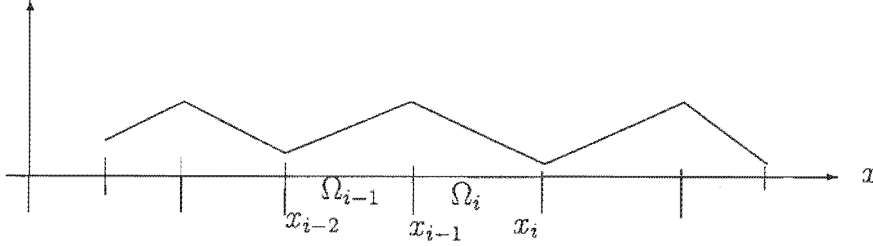


Figure 5.1: Shape functions for linear elements

### Variational formulation

The variational formulation of the problem (5.1) is as follows: find a function  $u$  that belongs to  $H^1(\Omega)$ , and that satisfies the equation

$$b(u, v) = L(v) \text{ for all } v \in H^1(\Omega). \quad (5.16)$$

Here  $b(.,.)$  is the bilinear form and  $L$  the linear functional defined by

$$b(u, v) = \left( \beta \frac{du}{dx} + u, v \right) \quad (5.17)$$

and

$$L(v) = (f, v), \quad (5.18)$$

where  $(.,.)$  denotes the  $L^2$ -inner product on  $\Omega$ .

Equation (5.16) is obtained by multiplying (5.1) by the weight function  $v$  and integrating over  $\Omega$ .

**Definition 5.1** The bilinear form  $b(.,.)$  is said to be

(a) continuous if there exists  $M > 0$  such that for any  $u, v \in H^1(\Omega)$ ,

$$|b(u, v)| \leq M \|u\|_1 \|v\|_1; \quad (5.19)$$

(b)  $H^1$ -elliptic or coercive if there exists  $\alpha > 0$  such that

$$\alpha \|v\|_1^2 \leq b(v, v), \text{ for all } v \in H^1(\Omega). \quad (5.20)$$

**Lemma 5.1** For any  $v \in H^1(\Omega)$ , we have

$$b(v, v) = \frac{1}{2}|v|^2 + \|v\|^2, \quad (5.21)$$

where  $|v|$  is given by (5.13).

**Proof.** We have

$$b(v, v) = \left( \beta \frac{dv}{dx}, v \right) + (v, v). \quad (5.22)$$

By integrating by parts, we have

$$\begin{aligned} \left( \beta \frac{dv}{dx}, v \right) &= \int_a^b \beta \frac{dv}{dx} v \, dx \\ &= \left[ \beta v^2 \right]_a^b - \int_a^b v \beta \frac{dv}{dx} \, dx \\ &= \langle v, v \rangle - \left( v, \beta \frac{dv}{dx} \right), \end{aligned}$$

which gives

$$\left( \beta \frac{dv}{dx}, v \right) = \frac{1}{2} \langle v, v \rangle. \quad (5.23)$$

By substituting (5.23) in (5.22), we get the required result.  $\square$

### 5.1.2 Standard Galerkin method

The Standard Galerkin approximation of (5.16) is the problem of finding  $u^h \in V_h$  with  $u^h(a) = g$  such that

$$b(u^h, v) = L(v), \text{ for all } v \in V_h. \quad (5.24)$$

Subtracting (5.24) from (5.16), we get

$$b(e, v) = 0 \text{ for all } v \in V_h, \quad (5.25)$$

where

$$e = u - u^h \quad (5.26)$$

is the error between the exact solution and the finite element approximation.

**Proposition 5.1 (Céa's Lemma)** *Let  $V$  be a closed subspace of a Hilbert space, and let  $b(.,.)$  and  $L(.)$  be, respectively, a continuous  $V$ -elliptic bilinear form and a bounded linear functional on  $V$ . Then there exists a constant  $C$ , independent of  $h$ , such that*

$$\|u - u^h\|_V \leq C \inf_{v^h \in V_h} \|u - v^h\|. \quad (5.27)$$

**Proof.** We have

$$\begin{aligned} \alpha \|u - u^h\|_V^2 &\leq b(u - u^h, u - u^h), \text{ since } b(.,.) \text{ is } V\text{-elliptic} \\ &= b(u - u^h, u - v^h - u^h + v^h) \\ &= b(u - u^h, u - v^h) - b(e, u^h - v^h) \\ &= b(u - u^h, u - v^h), \text{ using (5.25)} \\ &\leq M \|u - u^h\| \|u - v^h\|, \text{ since } b(.,.) \text{ is continuous.} \end{aligned}$$

Thus

$$\|u - u^h\|_V \leq C_1 \|u - v^h\|,$$

where  $C_1 = \frac{M}{\alpha}$ .

Since  $b(u - u^h, w^h) = 0$  for all  $w^h \in V_h$ , it follows that  $u^h$  is the projection of the exact solution  $u$  onto  $V_h$ , in the inner product  $b(., .)$ . Therefore, we have

$$b(u - u^h, u - u^h) = \inf_{v^h \in V_h} b(u - v^h, u - v^h). \quad (5.28)$$

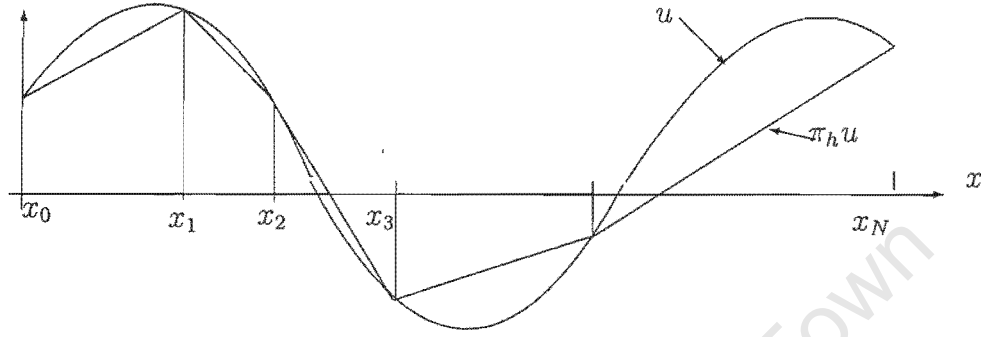
By using the V-ellipticity and the continuity of the bilinear form, we have

$$\|u - u^h\|_V \leq C \inf_{v^h \in V_h} \|u - v^h\|, \quad (5.29)$$

where  $C = \sqrt{\frac{M}{\alpha}}$ .  $\square$

**Remark 5.2** Céa's Lemma shows that the problem of evaluation of the error  $u - u^h$  can be transformed to a problem of approximation theory for evaluating the distance between  $u$  and  $V_h$ ; this is explained by the quantity  $\inf_{v^h \in V_h} \|u - v^h\|_{H^1(\Omega)}$ .

**Definition 5.2** If  $u$  is the exact solution of (5.16), the interpolate of  $u$  is a function  $\pi_h u$  in  $V_h$  whose value coincides with that of  $u$  at the  $N + 1$  points  $x_0, x_1, x_2, \dots, x_N$  in  $\Omega$  (see Figure 5.2).

Figure 5.2: The interpolate of  $u$ 

**Lemma 5.2 (Young's inequality)** *For any real numbers  $a$  and  $b$ , and  $\varepsilon > 0$ ,*

$$2ab \leq \varepsilon a^2 + \varepsilon^{-1} b^2. \quad (5.30)$$

**Proposition 5.2** *There is a constant  $C$  such that if  $u \in H^2(\Omega)$  satisfies (5.16) and  $u^h \in V_h$  is the solution of (5.24), then as  $h \rightarrow 0$ ,*

$$\|u - u^h\| + |u - u^h| \leq C h \|u\|_2. \quad (5.31)$$

**Proof.** Let  $\pi^h u$  be the interpolate of  $u$  and write  $\eta^h = u - \pi^h u$ , and  $e^h = u^h - \pi^h u$  so that  $e^h = \eta^h - e$ , where  $e = u - u^h$ . By using Lemma 5.1 and (5.25) with  $u = e^h$ , we have

$$\begin{aligned} b(e^h, e^h) &= b(\eta^h, e^h) - b(e, e^h) \\ &= b(\eta^h, e^h), \text{ using (5.25)} \end{aligned}$$

$$\begin{aligned}
&= \left( \beta \frac{d\eta^h}{dx} + \eta^h, e^h \right) \\
&= \left( \beta \frac{d\eta^h}{dx}, e^h \right) + (\eta^h, e^h) \\
&\leq \left\| \beta \frac{d\eta^h}{dx} \right\| \|e^h\| + \|\eta^h\| \|e^h\|, \\
&\text{using the Cauchy - Schwarz inequality} \\
&\leq \left\| \beta \frac{d\eta^h}{dx} \right\|^2 + \frac{1}{4} \|e^h\|^2 + \frac{1}{4} \|e^h\|^2 + \|\eta^h\|^2, \quad (5.32) \\
&\text{using Young's inequality with } \varepsilon = 2.
\end{aligned}$$

Substituting (5.22) in the LHS of (5.32), we have

$$\frac{1}{2} \|e^h\|^2 + \frac{1}{2} \|e^h\|^2 \leq \left\| \beta \frac{d\eta^h}{dx} \right\|^2 + \|\eta^h\|^2. \quad (5.33)$$

From finite element interpolation theory [24], we have

$$\left\| \beta \frac{d\eta^h}{dx} \right\| \leq C_1 h \|u\|_2, \quad (5.34)$$

$$\|\eta^h\| \leq C_1 h^2 \|u\|_2 \quad (5.35)$$

and

$$\|\eta^h\| \leq C_1 h^2 \|u\|_2, \quad (5.36)$$

with  $C_1$  a constant.

So we have

$$\begin{aligned}
\left\| \beta \frac{d\eta^h}{dx} \right\| + \|\eta^h\| &\leq C_1 h \|u\|_2 + C_1 h^2 \|u\|_2 \\
&= C_1 h (1 + h) \|u\|_2 \\
&= C_2 h \|u\|_2, \quad (5.37)
\end{aligned}$$

with  $C_2$  is a constant, if  $0 < h < 1$ .

Now the continued inequality

$$(a + b)^2 \leq 2(a^2 + b^2) \leq 2(c^2 + d^2) \leq 2(c + d)^2 \quad (5.38)$$

implies that

$$(a + b) \leq \sqrt{2}(c + d), \quad (5.39)$$

for real numbers  $a, b, c$  and  $d$ . Using (5.37), (5.38) and (5.39), (5.33), we get

$$\|e^h\| + |e^h| \leq Ch\|u\|_2, \quad (5.40)$$

where  $C$  is a constant.

Since

$$\|\eta^h\| + |\eta^h| \leq Ch^2\|u\|_2, \quad (5.41)$$

adding (5.40) and (5.41), we have

$$\|e^h\| + \|\eta^h\| + |e^h| + |\eta^h| \leq Ch\|u\|_2. \quad (5.42)$$

On the other hand, using  $e = e^h - \eta^h$  and using the triangle inequality, we have

$$\|e\| \leq \|e^h\| + \|\eta^h\|, \quad (5.43)$$

$$|e| \leq |e^h| + |\eta^h|, \quad (5.44)$$

so that

$$\begin{aligned} \|e\| &\leq Ch\|u\|_2 + Ch^2\|u\|_2 \\ &\leq Ch\|u\|_2. \end{aligned} \quad (5.45)$$

Similarly,

$$|e| \leq Ch\|u\|_2, \quad (5.46)$$

so that we have

$$\|e\| + |e| \leq Ch\|u\|_2. \quad (5.47)$$

□

**Corollary 5.1** *There is a constant  $C$  such that if  $u \in H^2(\Omega)$  satisfies (5.16) and  $u^h \in V_h$  is the solution of (5.24), then as  $h \rightarrow 0$ ,*

$$\|u - u^h\| \leq C h \|u\|_2. \quad (5.48)$$

**Remark 5.3** Proposition 5.2 shows that the error for the Galerkin method is not optimal, in that one would expect an error of  $O(h^2)$ .

### 5.1.3 Streamline Upwind (SU) Method

As we stated at the beginning of this chapter, because of the convective term in our problem, the standard finite element method does not give good approximation. We showed that the error for the Galerkin method is of  $O(h)$ , which is not optimal [7]. In addition, this estimate requires that  $u \in H^2(\Omega)$ . We would like to improve the rate of convergence by using a non-standard finite element method. Here we consider the streamline upwind method; we follow the work of Tanner and Jin [34].

The Streamline Upwind (SU) approximation of problem (5.1) is that of finding  $u^h \in V_h$  such that

$$\int_a^b \left( \beta \frac{du^h}{dx} \right) \ell \frac{dw^h}{dx} dx + \int_a^b \left( \beta \frac{du^h}{dx} + u^h - f \right) w^h dx = 0 \quad (5.49)$$



for all  $w^h \in V_h$ , where  $\ell$  is a piecewise constant function that varies from element to element.

If  $u$  is the exact solution of (5.16), then for any  $w^h$ , we have

$$\int_a^b \left( \beta \frac{du}{dx} + u - f \right) w^h dx = 0. \quad (5.50)$$

Choose  $w_h$  to be the basis function satisfying  $w_h(x_i) = 1$  and  $w_h = 0$  at all other nodes. We choose also  $\ell = \frac{h_i}{2}$ ; then  $\frac{dw^h}{dx} = \frac{1}{h_i}$  on  $\Omega_{i-1}$  and equal to  $-\frac{1}{h_i}$  on  $\Omega_i$ . Replacing  $w^h$  by  $w = w^h + \ell \frac{dw^h}{dx}$  in (5.50), we get

$$\int_a^b \left[ \left( \beta \frac{du}{dx} + u - f \right) w^h + \left( \beta \frac{du}{dx} + u - f \right) \ell \frac{dw^h}{dx} \right] dx = 0 \quad (5.51)$$

Subtracting (5.49) from (5.51), we get

$$\int_a^b \left( \beta \frac{de}{dx} + e \right) \left( w^h + \ell \frac{dw^h}{dx} \right) dx = - \int_a^b (u^h - f) \ell \frac{dw^h}{dx} dx. \quad (5.52)$$

We now study the special limiting case  $\beta \rightarrow \infty$ , for which  $u \rightarrow 0$  (see (5.3)). In the limit, the error equation (5.52) becomes

$$\int_a^b \beta \frac{de}{dx} \left( w^h + \ell \frac{dw^h}{dx} \right) dx \approx \int_a^b f \ell \frac{dw^h}{dx} dx. \quad (5.53)$$

Assuming that  $f$  is continuous and differentiable near  $x_i$ ,  $f$  may be expanded according to

$$f = f_i + (x - x_i)f'_i + O(x - x_i)^2, \quad (5.54)$$

where  $f_i = f(x_i)$ .

The right hand side of (5.53) is therefore, using also  $\ell_i \frac{dw^h}{dx} = \pm 0.5$ ,

$$\begin{aligned}
 & \int_{\Omega} \left[ f_i + (x - x_i) f'_i + O((x - x_i)^2) \right] \pm 0.5 \, dx \\
 &= \int_{x_{i-1}}^{x_i} \left[ f_i + (x - x_i) f'_i + O((x - x_i)^2) \right] \frac{1}{2} dx \\
 &\quad - \int_{x_i}^{x_{i+1}} \left[ f_i + (x - x_i) f'_i + O((x - x_i)^2) \right] \frac{1}{2} dx \\
 &= -\frac{1}{2} f_i (h_i - h_{i-1}) - \frac{1}{4} f'_i (h_{i-1}^2 + h_i^2) + O(h^3) .
 \end{aligned}$$

The LHS of (5.53) becomes

$$\begin{aligned}
 \int_a^b \beta \frac{de}{dx} (w^h \pm 0.5) \, dx &= \beta \frac{de}{dx} (\xi_{i-1}) \int_{x_{i-1}}^{x_i} (w^h + 0.5) \, dx \\
 &\quad + \beta \frac{de}{dx} (\xi_i) \int_{x_i}^{x_{i+1}} (w^h - 0.5) \, dx \\
 &= \beta \frac{de}{dx} (\xi_{i-1}) (0.5 h_{i-1} + 0.5 h_{i-1}) \\
 &\quad + \beta \frac{de}{dx} (\xi_i) (0.5 h_i - 0.5 h_i) \\
 &= \beta \frac{de}{dx} \Big|_{\xi_{i-1}} h_{i-1} , \tag{5.55}
 \end{aligned}$$

by using the mean value theorem, where  $\xi_{i-1}$  and  $\xi$  are respectively points in  $\Omega_{i-1}$  and  $\Omega_i$ .

So one can write (5.53) as

$$\beta \left( \frac{de}{dx} \right)_{-} h_{i-1} \approx -\frac{1}{2} f_i (h_i - h_{i-1}) - \frac{1}{4} f'_i (h_{i-1}^2 + h_i^2) + O(h^3) , \tag{5.56}$$

where  $\left(\frac{de}{dx}\right)_-$  lies on the left-hand element (see Figure 5.1).

For  $h_i \neq h_{i-1}$  (unequal elements), using the fact that  $f_i \approx \beta \frac{du}{dx}$ , and  $f'_i = \beta \frac{d^2u}{dx^2}$ , (5.56) becomes

$$\left(\frac{de}{dx}\right)_- \approx -\frac{1}{2} \left(\frac{du}{dx}\right)_i \frac{h_i - h_{i-1}}{h_{i-1}} + O(h^2), \quad (5.57)$$

so the error in the slope is of the same order as the slope of the exact solution.

For  $h_i = h_{i-1}$  (equal elements), then from (5.56) and using (5.3), we have the slope of the error is of order  $h$  and

$$\left(\frac{de}{dx}\right)_- \approx -\frac{1}{2} \left(\frac{d^2u}{dx^2}\right)_i h_i + O(h^2), \quad (5.58)$$

so that the error in the slope is of order  $O(h)$ .

This is illustrated in Figure 5.3 below.

From Figure 5.3, we have

$$\left.\frac{de}{dx}\right|_- \approx Ch. \quad (5.59)$$

Now  $\frac{de}{dx}$  is continuous and bounded in  $\Omega_{i-1}$ , so that  $\left|\frac{de}{dx}\right| \leq Ch$ , and

from (5.59) we have  $\left\|\frac{de}{dx}\right\| \leq Ch$ . Thus we have

$$\left\|\frac{de}{dx}\right\| \leq Ch \left\|\frac{d^2u}{dx^2}\right\|. \quad (5.60)$$

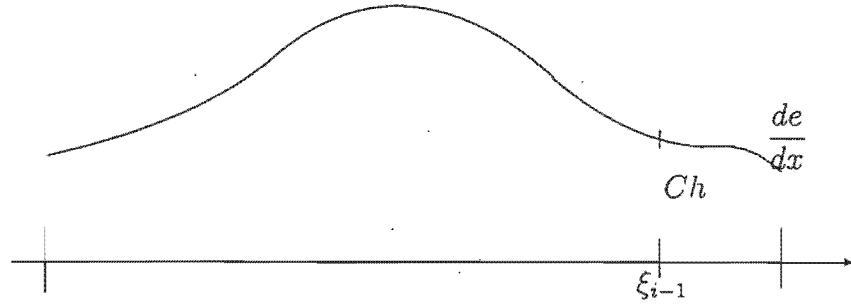


Figure 5.3: The error in the slope

Suppose now that  $f$  is piecewise constant, with  $f|_{\Omega_i} = f_i = \text{constant}$ ; then the RHS of (5.53) becomes

$$\frac{1}{2} \int_{x_{i-1}}^{x_i} f_{i-1} dx - \frac{1}{2} \int_{x_i}^{x_{i+1}} f_i dx = \frac{1}{2} (f_{i-1} h_{i-1} - f_i h_i) \quad (5.61)$$

and the LHS is

$$\beta \left( \frac{de}{dx} \right)_- h_{i-1}, \quad (5.62)$$

so that we have

$$\left( \frac{de}{dx} \right)_- = \frac{f_{i-1} h_{i-1} - f_i h_i}{h_{i-1}}. \quad (5.63)$$

We conclude that

$$\left( \frac{de}{dx} \right)_- = O(1), \quad (5.64)$$

so that the slope of the error is of  $O(1)$  in general, that is, for both uniform and non-uniform meshes.

Next we find an estimate for  $\|e\|$ . Consider the general problem (5.49) and (5.50), and take  $w^h = e$ ; then (5.50) becomes

$$\int_a^b \left( \beta \frac{du}{dx} + u - f \right) e \, dx = 0. \quad (5.65)$$

Subtracting (5.49) from (5.65), we obtain

$$\int_a^b \left( \beta \frac{de}{dx} + e \right) e \, dx = \frac{\beta}{2} \int_a^b \left( \frac{du}{dx} - \frac{de}{dx} \right) \frac{de}{dx} h_i \, dx, \quad (5.66)$$

by substituting

$$\frac{du^h}{dx} = \frac{du}{dx} - \frac{de}{dx}. \quad (5.67)$$

Equation (5.66) is equivalent to

$$\int_a^b \beta \frac{de}{dx} e \, dx + \int_a^b e^2 \, dx + \frac{\beta}{2} \int_a^b \left( \frac{de}{dx} \right)^2 \ell \, dx = \frac{\beta}{2} \ell \int_a^b \frac{du}{dx} \frac{de}{dx} \, dx, \quad (5.68)$$

which can be also written as

$$\frac{1}{2} \beta \int_a^b \frac{d}{dx} (e^2) \, dx + \int_a^b e^2 \, dx + \frac{\beta}{2} \int_a^b \left( \frac{de}{dx} \right)^2 \ell \, dx = \frac{\beta}{2} \int_a^b \frac{du}{dx} \frac{de}{dx} \ell \, dx. \quad (5.69)$$

After using the Cauchy-Schwarz inequality, (5.69) becomes

$$\frac{1}{2} \beta e^2(b) - \frac{1}{2} \beta e^2(a) + \|e\|^2 + \beta \frac{h_{\min}}{2} \left\| \frac{de}{dx} \right\|^2 \leq \beta \frac{h_{\max}}{2} \left\| \frac{du}{dx} \right\| \left\| \frac{de}{dx} \right\|. \quad (5.70)$$

Let us assume that the error vanishes at  $\Gamma_-$ , due to the boundary condition. From (5.70), we have

$$\|e\|^2 \leq \frac{h_{max}}{2} \left\| \frac{du}{dx} \right\| \left\| \frac{de}{dx} \right\|. \quad (5.71)$$

For the case of a uniform mesh,  $\left\| \frac{de}{dx} \right\|$  is of  $O(h)$  as in (5.60), so that (5.71) becomes

$$\|e\| \leq C_1 h, \quad (5.72)$$

For non-uniform meshes, (5.70) implies that

$$\beta \frac{h_{min}}{2} \left\| \frac{de}{dx} \right\|^2 \leq \frac{h_{max}}{2} \left\| \frac{du}{dx} \right\| \left\| \frac{de}{dx} \right\|. \quad (5.73)$$

By assuming that  $\frac{h_{max}}{h_{min}} \leq C$  (see, [7]), we have

$$\left\| \frac{de}{dx} \right\| \leq C \left\| \frac{du}{dx} \right\| \quad (5.74)$$

with  $C$  is a constant. Thus the error in the slope does not go to zero as  $h \rightarrow 0$ .

If  $f$  is constant and the mesh is uniform, then (5.71) implies that

$$\|e\| \leq C_2 h^{\frac{1}{2}} \left\| \frac{du}{dx} \right\|, \text{ where } C_2 \text{ is a constant,} \quad (5.75)$$

since the slope of the error is of  $O(1)$ , (see (5.64)).

We can now summarise the results as follows :

### Summary

For  $\beta \rightarrow \infty$  and  $f$  not a constant, we have

$$\left\| \frac{du}{dx} - \frac{du^h}{dx} \right\| \leq C \left\| \frac{du}{dx} \right\| \quad (\text{non-uniform meshes}) \quad (5.76)$$

$$\left\| \frac{du}{dx} - \frac{du^h}{dx} \right\| \leq C h \left\| \frac{d^2u}{dx^2} \right\| \quad (\text{uniform meshes}) \quad (5.77)$$

$$\|u - u^h\| \leq C h^{\frac{1}{2}} \left\| \frac{du}{dx} \right\| \quad (\text{non-uniform meshes}) \quad (5.78)$$

$$\|u - u^h\| \leq C h \left\| \frac{d^2u}{dx^2} \right\| \quad (\text{uniform meshes}) \quad (5.79)$$

We can thus conclude that the norm of the error in the SU scheme is  $O(h)$  in the case of uniform meshes and is  $O(h^{\frac{1}{2}})$  in the case of non-uniform meshes for high value of  $\beta$ .

For  $f$  a constant and  $\beta \rightarrow \infty$ , we have found that  $\frac{de}{dx}$  is of  $O(1)$  in case of uniform or non-uniform meshes, and  $\|e\| \leq C h^{1/2} \left\| \frac{du}{dx} \right\|$  for non-uniform meshes.

#### 5.1.4 Streamline Upwind Petrov/Galerkin (SUPG) method

In this subsection we will follow the work of Johnson [24]. The Streamline Upwind Petrov/Galerkin approximation of (5.1) is to find  $u^h \in V_h$  such that

$$\left( \beta \frac{du^h}{dx} + u^h - f, w + \beta \frac{dw}{dx} h \right) - (1+h) \langle u^h, w \rangle_- = -(1+h) \langle g, w \rangle_-, \quad (5.80)$$

for all  $w \in V_h$ . Let us introduce the notation

$$B(u, w) = \left( \beta \frac{du}{dx} + u, w + \beta \frac{dw}{dx} h \right) - (1+h) \langle u, w \rangle_- \quad (5.81)$$

and

$$L(w) = \left( f, w + \beta \frac{dw}{dx} h \right) - (1+h) \langle g, w \rangle_- . \quad (5.82)$$

Then (5.80) can be formulated as follows: find  $u^h \in V_h$  such that

$$B(u^h, w) = L(w), \text{ for all } w \in V_h. \quad (5.83)$$

Moreover, the exact solution of (5.1) satisfies

$$B(u, w) = L(w), \text{ for all } v \in V_h. \quad (5.84)$$

Subtracting (5.83) from (5.84), we have the usual orthogonality relation

$$B(e, w) = 0 \text{ for all } w \in V_h \quad (5.85)$$

for the error.

We define the norm

$$\|w\|_\beta = \left( h \left\| \beta \frac{dw}{dx} \right\|^2 + \|w\|^2 + \frac{1+h}{2} |w|^2 \right)^{\frac{1}{2}}. \quad (5.86)$$

**Lemma 5.3** *For any  $v \in H^1(\Omega)$  we have*

$$B(v, v) = \|v\|_\beta^2. \quad (5.87)$$



**Proof.**

$$\begin{aligned}
B(v, v) &= \left( \beta \frac{dv}{dx} + v, v + \beta \frac{dv}{dx} h \right) - (1 + h) \langle v, v \rangle_- \\
&= \left( \beta \frac{dv}{dx}, v \right) + \left( \beta \frac{dv}{dx}, \beta \frac{dv}{dx} h \right) + (v, v) + h \left( v, \beta \frac{dv}{dx} \right) \\
&\quad - (1 + h) \langle v, v \rangle_- \\
&= \left( \beta \frac{dv}{dx}, v \right) + h \left( \beta \frac{dv}{dx}, \beta \frac{dv}{dx} \right) + \|v\|^2 + h \left( v, \beta \frac{dv}{dx} \right) \\
&\quad - (1 + h) \langle v, v \rangle_- \\
&= (1 + h) \left( v, \beta \frac{dv}{dx} \right) + h \left\| \beta \frac{dv}{dx} \right\|^2 + \|v\|^2 \\
&\quad - (1 + h) \langle v, v \rangle_- \\
&= h \left\| \beta \frac{dv}{dx} \right\|^2 + \|v\|^2 \\
&\quad + \frac{1 + h}{2} \langle v, v \rangle - (1 + h) \langle v, v \rangle_-, \text{ using (5.23)} \\
&= \frac{1 + h}{2} (\langle v, v \rangle_+ + \langle v, v \rangle_-) + h \left\| \beta \frac{dv}{dx} \right\|^2 + \|v\|^2 \\
&\quad - (1 + h) \langle v, v \rangle_-, \\
&\text{using (5.14)} \\
&= \frac{1 + h}{2} |v|^2 + \|v\|^2 + h \|v\|_\beta^2, \tag{5.88}
\end{aligned}$$

which proves the desired equality.  $\square$

**Theorem 5.1** *There is a constant  $C$  such that if  $u^h$  satisfies (5.80), then*

$$\|u - u^h\|_\beta \leq C h^{3/2} \|u\|_2. \tag{5.89}$$

**Proof.** Let  $\pi_h u$  be the interpolate of  $u$ ,  $\eta^h = u - \pi_h u$  and  $e^h = u^h - \pi_h u$ . Using Lemmas 5.3 and (5.85), we get

$$\|e\|_\beta = B(e, e)$$

$$\begin{aligned}
&= B(e, \eta^h) - b(e, e^h) \\
&= B(e, \eta^h), \text{ using (5.25)} \\
&= \left( \beta \frac{de}{dx} + e, \eta^h + \beta \frac{d\eta^h}{dx} h \right) - (1+h) \langle e, \eta^h \rangle_- \\
&= \left( \beta \frac{de}{dx}, \eta^h \right) + h \left( \beta \frac{de}{dx}, \beta \frac{d\eta^h}{dx} \right) + (e, \eta^h) + h \left( e, \beta \frac{d\eta^h}{dx} \right) \\
&\quad - (1+h) \langle e, \eta^h \rangle_- \\
&\leq \left\| \beta \frac{de}{dx} \right\| \|\eta^h\| + h \left\| \beta \frac{de}{dx} \right\| \left\| \beta \frac{d\eta^h}{dx} \right\| + \|e\| \|\eta^h\| + h \|e\| \left\| \beta \frac{d\eta^h}{dx} \right\| \\
&\quad + (1+h) |e| |\eta^h|, \\
&\quad \text{using the Schwarz inequality} \\
&\leq \frac{h}{4} \left\| \beta \frac{de}{dx} \right\|^2 + h^{-1} \|\eta^h\|^2 + \frac{h}{4} \left\| \beta \frac{de}{dx} \right\|^2 + h \left\| \beta \frac{d\eta^h}{dx} \right\|^2 + \frac{1}{4} \|e\|^2 \\
&\quad + \|\eta^h\|^2 + \frac{1}{4} \|e\|^2 + h^2 \left\| \beta \frac{d\eta^h}{dx} \right\|^2 + \frac{1+h}{4} |e|^2 + (1+h) |\eta^h|^2, \\
&\hspace{25em} (5.90)
\end{aligned}$$

Using the Young's inequality (5.30) with  $\varepsilon = h/2$  in the first and fourth term and  $\varepsilon = 2$  in the second and third term, (5.90) becomes

$$\begin{aligned}
\|e\|_\beta &\leq \frac{h}{2} \left\| \beta \frac{de}{dx} \right\|^2 + \frac{1}{2} \|e\|^2 + (1+h^{-1}) \|\eta^h\|^2 (h+h^2) \left\| \beta \frac{d\eta^h}{dx} \right\|^2 \\
&\quad + \frac{1+h}{4} |e|^2 + (1+h) |\eta^h|^2. \\
&\hspace{25em} (5.91)
\end{aligned}$$

Using (5.86) in the LHS of (5.91), we have

$$\begin{aligned}
h \left\| \beta \frac{de}{dx} \right\|^2 + \|e\|^2 + \frac{1+h}{2} |e|^2 &\leq \frac{h}{2} \left\| \beta \frac{de}{dx} \right\|^2 + \frac{1}{2} \|e\|^2 + (1+h^{-1}) \|\eta^h\|^2 \\
&\quad + (h+h^2) \left\| \beta \frac{d\eta^h}{dx} \right\|^2 + \frac{1+h}{4} |e|^2 \\
&\quad + (1+h) |\eta^h|^2,
\end{aligned}$$

which gives

$$\frac{1}{2} \|e\|_{\beta}^2 \leq (1 + h^{-1}) \|\eta^h\|^2 + (h + h^2) \left\| \beta \frac{d\eta^h}{dx} \right\|^2 + (1 + h) |\eta^h|^2 \quad (5.92)$$

From finite element interpolation theory [24], we have

$$\begin{aligned} \|\eta^h\| &\leq C_1 h^2 \|u\|_2, \\ \left\| \beta \frac{d\eta^h}{dx} \right\| &\leq C_1 h \|u\|_2, \\ |\eta^h| &\leq C_1 h^{3/2} \|u\|_2; \end{aligned} \quad (5.93)$$

thus

$$\|e\|_{\beta}^2 \leq C_1 h^3 (1 + h) \|u\|_2^2, \quad (5.94)$$

which implies that

$$\|e\|_{\beta} \leq C_2 h^{3/2} \|u\|_2, \quad (5.95)$$

with  $C$  a constant.

Using (5.86) and (5.95), we get

$$\|e\| \leq C h^{3/2} \|u\|_2, \quad (5.96)$$

which is the desired result.  $\square$

## 5.2 Application to unidirectional flow of fibre suspensions

As in the last section of Chapter 4, we replace  $\mathbf{A}$  by  $\tilde{\mathbf{A}}$ , so that we can accommodate the limiting case  $\tilde{\mathbf{A}} \rightarrow \mathbf{0}$  as  $\gamma \rightarrow \infty$ . Then our problem can be written as (4.12), and solutions are sought in the space

$$\tilde{\Lambda} = \{ \tilde{A}_{ij} \in H^1(\Omega) : \tilde{A}_{ij} = \tilde{A}_{ji} \text{ and } \tilde{A}_{ii} = 0 \}. \quad (5.97)$$

### (a) Theoretical error

Recall that the equation for the unidirectional flow is

$$\gamma \frac{d\tilde{\mathbf{A}}}{dx} + 3\tilde{\mathbf{A}} = \mathbf{f}, \quad (5.98)$$

with  $\mathbf{f} = \mathbf{I} - 3\mathbf{A}^*$ .

For simplification, we will write  $\mathbf{A}$  instead of  $\tilde{\mathbf{A}}$

Note that (5.98) is similar to (5.1), with  $f$  a constant. Assuming that the elements are piecewise linear, we can then apply the results that we found in the previous sections. So we have:

#### (a.1) Galerkin method

$$\|\mathbf{A} - \mathbf{A}^h\| \leq C h^{\frac{3}{2}} \|\mathbf{A}\|_2 \quad (5.99)$$

#### (a.2) SUPG

$$\|\mathbf{A} - \mathbf{A}^h\| \leq C h^{\frac{3}{2}} \|\mathbf{A}\|_2 \quad (5.100)$$

(a.3) SU The error and the slope of the error for SU are of  $O(1)$  for non-uniform meshes and  $\|e\| \leq Ch^{1/2}$  for uniform meshes.

# Chapter 6

## Conclusions

In this work, we have considered the question of what types of restrictions are placed on the constitutive equations for fibre suspensions, by the second law of thermodynamics. The model investigated is that based on the use of the orientation tensor together with a closure approximation, and the study has focussed on restrictions on the constitutive equations, for two different closures, viz. the linear and quadratic closure approximations.

We have shown that, if the particle number is bounded according to  $N_p \leq \frac{35}{2}$ , then the constitutive equations with the linear closure approximations are consistent with the second law, and flows using this closure are monotonically and exponentially stable in an energetic sense. We have also shown shown that the quadratic closure is consistent with the second law, and flows obtained with this closure are monotonically and exponentially stable.

The second part of this thesis has been concerned with one-dimensional fibre suspension flows. In particular, theoretical error estimates for finite element approximations are studied, first for a general class of

boundary-value problems, after which the results are applied to the case of unidirectional flows. Because of the presence of convective terms, it is necessary to make use of non-standard finite element methods in order to obtain convergence at optimal rates. The methods studied are the Streamline Upwind (SU) method and the Streamline Upwind Petrov-Galerkin (SUPG) method. It is found that in the case where  $f$  is not a constant, the norm in the error in the orientation tensor for the SU scheme is  $O(h)$  for uniform meshes, and  $O(h^{\frac{1}{2}})$  for non-uniform meshes and for high values of the Weissenberg-like parameter  $\gamma$ , and when  $f$  is a constant the norm in the error in the orientation tensor for the SU scheme is  $O(h^{1/2})$  for non-uniform mesh and the norm of the slope of the error in the orientation tensor is of  $O(1)$  for uniform and non-uniform meshes. We also found that the error  $de/dx$  does not go to zero as  $h \rightarrow 0$ , which means that there is no convergence (see (5.74)).

For the SUPG method, the error is  $O(h^{\frac{3}{2}})$  for the case of SUPG and the error is  $O(h^{\frac{3}{2}})$  for the Galerkin method.

Much work remains to be done in this area. First, it would be interesting to investigate the consistency of a wider range of closure approximations with the second law. Secondly, it would be useful to extend the finite element analysis to include non-homogenous boundary value problems, such as that arising in the case of radial flows. And of course, it remains to study numerical simulations, and to compare the errors obtained in this way with the estimates in the thesis.

# Appendix A

## Some useful properties

**Proposition A.1** *Let tensor  $D$  be the symmetric part of any tensor  $L$ . If  $A$  is a symmetric tensor, then*

$$A : L = A : D , \quad (\text{A.1})$$

### Proof

Set  $L = D + W$ , in which  $D$  (resp  $W$ ) is the symmetric (resp the skew) part of tensor  $L$ .

The fact that  $A$  is symmetric and  $W$  is the skew part of  $L$  implies that  $A : W = 0$ .

So, we have:

$$\begin{aligned} A : L &= A : (D + W) \\ &= A : D . \end{aligned}$$

**Proposition A.2** *For any two symmetric tensors  $D$  and  $A$ , the following assertion holds*

$$(A \otimes A)D = A(A : D) . \quad (\text{A.2})$$

**Proof**

$$\begin{aligned}
 (A \otimes A)D &= (A_{ij}A_{kl})D_{kl} \\
 &= A_{ij}(A_{kl}D_{kl}) \\
 &= A(A : D) .
 \end{aligned}$$

**Corollary A.1** *For any three tensors  $A$ ,  $D$  and  $L$  which satisfy the conditions of Propositions A.1 and A.2, the following relation holds :*

$$(A \otimes A)D : L = (A : D)^2 . \quad (\text{A.3})$$

**Proof**

$$\begin{aligned}
 (A \otimes A)D : L &= A(A : D) : L \\
 &= (A : D)(A : L) \\
 &= (A : D)^2 ,
 \end{aligned}$$

since  $A$  is symmetric

**Corollary A.2** *For any three tensors  $A$ ,  $D$  and  $L$  which satisfy the conditions of Proposition A.1. The following relation holds*

$$DA : L + AD : L = 2A : D^2 \quad (\text{A.4})$$

**Proof**

$$\begin{aligned}
 DA : L + AD : L &= (DA + AD) : L \\
 &= \left( DA + (DA)^T \right) : D \\
 &= A : D^2 + A : D^2 \\
 &= 2A : D^2
 \end{aligned}$$



# Appendix B

## Some mathematical definitions

**Definition B.1** Let  $V$  be a linear space.  $L : V \rightarrow \mathbb{R}, L(v) \in \mathbb{R}$  for all  $v \in V$ , is a linear form if and only if

$$L(\beta v + \theta w) = \beta L(v) + \theta L(w), \quad (\text{B.1})$$

for all  $v, w \in V$

**Definition B.2** Let  $a : V \times V \rightarrow \mathbb{R}$  such that  $a(v, w) \in \mathbb{R}$  for  $v, w \in V$ .  $a$  is a bilinear form on  $V \times V$  if for all  $u, v, w \in V$  and  $\beta, \theta \in \mathbb{R}$ , we have

$$a(u, \beta v + \theta w) = \beta a(u, v) + \theta a(u, w) \quad (\text{B.2})$$

and

$$a(\beta u + \theta v, w) = \beta a(u, w) + \theta a(v, w) \quad (\text{B.3})$$

**Definition B.3** The bilinear form  $a(.,.)$  on  $V \times V$  is symmetric if

$$a(u, v) = a(v, u), \quad (\text{B.4})$$

for all  $u, v \in V$

**Definition B.4** A symmetric bilinear form  $a(.,.)$  on  $V \times V$  is said to be a scalar product on  $V$  if

$$a(v, v) \geq 0 \text{ for all } v \in V, v \neq 0 \quad (\text{B.5})$$

And the norm  $\|.\|_a$  associated to a scalar product  $a(.,.)$  is defined by

$$\|v\|_a = (a(v, v))^{\frac{1}{2}}, \text{ for all } v \in V \quad (\text{B.6})$$

**Proposition B.1** Let  $\langle ., . \rangle$  be a scalar product with corresponding norm  $\|.\|$ . Then the Cauchy's inequality states that

$$|\langle v, w \rangle| \leq \|v\| \|w\| \quad (\text{B.7})$$

**Definition B.5** Let  $V$  be a linear space with a scalar product with corresponding norm  $\|.\|$ .

$V$  is said to be a hilbert space if  $V$  is complete i.e. every Cauchy sequence with respect to  $\|.\|$  is convergent.

**Definition B.6** Let  $I = (a, b)$  be an interval. We define the space of "square integrable functions" on  $I$

$$L^2(I) = \left\{ v : v \text{ is defined on } I \text{ and } \int_I v^2 dx < \infty \right\} \quad (\text{B.8})$$

**Proposition B.2**  $L^2(I)$  is a Hilbert space with the scalar product

$$(v, w) = \int_I v w dx \quad (\text{B.9})$$

and corresponding norm

$$\|v\|_{L^2(I)} = \left( \int_I v^2 dx \right)^{\frac{1}{2}} = (v, v)^{\frac{1}{2}} \quad (\text{B.10})$$

**Definition B.7** Let  $I$  be an interval on  $\mathbb{R}$ . The Sobolev space  $H^1(I)$  is defined by

$$H^1(I) = \{v : v \in L^2(I) \text{ and } v' \in L^2(I)\}. \quad (\text{B.11})$$

$H^1(I)$  is a Hilbert space with inner product

$$(v, w)_{H^1(I)} = \int_I (vw + v'w') dx, \quad (\text{B.12})$$

and corresponding norm

$$\|v\|_{H^1(I)} = \left( \int_I [v^2 + (v')^2] dx \right)^{\frac{1}{2}}. \quad (\text{B.13})$$

**Definition B.8** Two norms  $\|\cdot\|$  and  $\|\cdot\|_+$  on  $H^k(\Omega)$  are equivalent iff there are positive constants  $c$  and  $d$  such that

$$c\|x\|_+ \leq \|x\| \leq d\|x\|_+, \text{ for all } x \in H^k(\Omega). \quad (\text{B.14})$$

**Theorem B.1 (Equivalent Norms Theorem [39])** Let  $\Omega$  be an open, bounded, connected set in  $\mathbb{R}^d$  with a Lipschitz boundary,  $k \geq 1$ . Assume that for  $1 \leq j \leq J$ ,  $f_j : H^k(\Omega) \rightarrow \mathbb{R}$ , are seminorms on  $H^k(\Omega)$  satisfying two conditions:

( $H_1$ )  $0 < f_j(v) \leq c\|v\|_k$  for all  $v \in H^k(\Omega)$ ,  $1 \leq j \leq J$ .

( $H_2$ ) If  $v$  is a polynomial of degree less than or equal to  $k - 1$  and  $f_j(v) = 0$ ,  $1 \leq j \leq J$ , then  $v = 0$ .

Then the quantity

$$\|v\| = |v|_k + \sum_{j=1}^J f_j(v) \quad (\text{B.15})$$

or

$$\|v\| = \left( |v|_k^2 + \sum_{j=1}^J f_j(v)^2 \right)^{1/2} \quad (\text{B.16})$$

defines a norm on  $H^k(\Omega)$ , which is equivalent to the norm  $\|v\|_k$ .

**Theorem B.2 (The Poincaré–Friedrichs inequality [32])** *Let  $\Omega$  be a bounded domain in  $\mathbb{R}^n$ . Then there exists a constant  $C > 0$  such that*

$$\int_{\Omega} |u|^2 dx \leq C \int_{\Omega} |\nabla u|^2 dx \quad \text{for all } u \in H_0^1(\Omega) \quad (\text{B.17})$$

**Theorem B.3 (Korn's first inequality [30])** *For  $v \in [H_0^1(\Omega)]^3$ , we define the tensor function*

$$\epsilon(v) = \frac{1}{2} (\nabla v + (\nabla v)^T).$$

*Korn's first inequality states that there exists a constant  $c > 0$  depending only on  $\Omega$  such that*

$$\|v\|_{[H^1(\Omega)]^3}^2 \leq c \int_{\Omega} |\epsilon(v)|^2 dx \quad \text{for all } v \in [H^1(\Omega)]^3. \quad (\text{B.18})$$

*We deduce from Korn's inequality and Equivalent Norms Theorem (Theorem B.1) that the norms  $\|v\|_{[H^1(\Omega)]^3}^2$  and  $\int_{\Omega} |\nabla v| dx = \|v\|$  are equivalent.*

*So if  $v \in [H^1(\Omega)]^3 \equiv \mathbb{H}^3(\Omega)$  from Sobolev's Inequalities, we may conclude that*

$$\int_{\Omega} \|D\|_{\mathbb{H}^3(\Omega)}^2 dx = \int_{\Omega} \|\epsilon(v)\|_{\mathbb{H}^3(\Omega)}^2 dx \leq c \|v\|_{\mathbb{H}^3(\Omega)}$$

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